New correlated-effective-field theory in the Ising model

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A new method incorporating the effects of many-body static spin correlations into an effective-field theory is discussed. The method is based on the introduction of a differential operator and the concept of the correlated effective field into two exact Callen identities of the Ising model. The resulting statistical theory is shown to have an accuracy equivalent to that of the Bethe-Peierls method. It is shown that the correlated-effective-field parameter at the transition temperature has a universal function of $1/(z-1)$, where z is the number of nearest neighbors.

The Ising problem has been one of the most actively studied problems in statistical mechanics. Rigorous solutions have been given for the simple model for one-dimensional and certain two-dimensional lattices.[1] There is also the series-expansion method which is valid for temperatures either very high or very low compared with the transition temperature.[2]

On the other hand, the first step in the interpretation of the magnetic properties of solids is usually the application of an effective-field theory. The theory can be relied on for an appropriate description of the major aspects of the phenomena being studied. However, the theory has some deficiencies, such as the neglect of the effects of short-range order. Improvements in this respect have been sought by many methods.[3]

A method of incorporating the effects of many-body static spin correlations in the effective-field theory has been discussed by Lines, in which he introduced the concept of a correlated effective field.[4] The correlated-effective-field parameter is determined at the end of the calculation by imposing consistency of the theory with a sum rule for the susceptibility. The correlated-effective-field approximation developed by Lines has been applied to a number of problems in magnetic systems.[5] However, the method gives an accuracy essentially equivalent to that of the spherical model, and unfortunately the sum rule is valid often only in the paramagnetic phase and in the absence of strong fields.

In this Communication we show a new approach for an effective-field theory with correlations, including the concept of the correlated effective field. Our method is based on the introduction of a differential operator into two exact Callen's identities of the Ising model, which gives a better result for a transition temperature than Line's method and is expected to have wide applications for problems in crystalline and disordered Ising magnets. In contrast with Line's results the resulting statistical theory is shown to have an accuracy equivalent to that of the Bethe-Peierls method,[3] although the principle and approach of our formulation are very different from the Bethe-Peierls method. It is shown that the correlated-effective-field parameter at the transition temperature has a universal function given by $1/(z-1)$, where z is the number of nearest neighbors.

The system consists of N identical spins, $\mu_i = \pm 1$, arranged on a lattice. The Hamiltonian is given by

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} J_{ij} \mu_i \mu_j \ , \tag{1}$$

where J_{ij} is the exchange interaction with $J_{ii} = 0$.

Formally, Callen[6] obtained an exact spin-correlation function as follows:

$$\langle \mu_i \rangle = \langle \tanh(\beta E_i) \rangle \tag{2}$$

with

$$E_i = \sum_j J_{ij} \mu_j \ ,$$

where $\langle \cdots \rangle$ indicates an ensemble average

$$\langle A \rangle = \frac{\mathrm{Tr} A e^{-\beta H}}{\mathrm{Tr} e^{-\beta H}} \ .$$

In previous papers,[7] we introduced the method of differential operator into Eq. (2) and discussed a new type of effective-field theory. The formalism has been applied to several problems of crystalline and

disordered Ising magnets. Therefore, let us introduce the differential operator into Eq. (2) as follows:

$$\langle \mu_i \rangle = \left\langle \exp\left(D \sum_j t_{ij}\mu_j\right)\right\rangle \tanh x|_{x=0}$$
$$= \left\langle \prod_j [\cosh(Dt_{ij}) + \mu_j \sinh(Dt_{ij})]\right\rangle \tanh x|_{x=0} , \quad (3)$$

with

$$t_{ij} = \frac{J_{ij}}{k_B T} ,$$

where

$$D = \frac{\partial}{\partial x} .$$

In order to clarify here how the concept of the correlated field is introduced into the present formulation, we restrict the discussions to the simple case of a square lattice with nearest-neighbor interactions J. Then, Eq. (3) reduces to

$$\langle \mu_i \rangle = K_1 \sum_{\delta=1}^{4} \langle \mu_{i+\delta}\rangle + \frac{K_2}{3!} \sum_{\delta_1} \sum_{\delta_2 (\neq \delta_1)} \sum_{\delta_3 (\neq \delta_1, \delta_2)} \langle \mu_{i+\delta_1}\mu_{i+\delta_2}\mu_{i+\delta_3}\rangle , \quad (4)$$

$$K_1 = \sinh(Dt)[\cosh(Dt)]^3 \tanh x|_{x=0}$$
$$= \tfrac{1}{8}[\tanh(4t) + 2\tanh(2t)] , \quad (5)$$

and

$$K_2 = [\sinh(Dt)]^3 \cosh(Dt) \tanh x|_{x=0}$$
$$= \tfrac{1}{8}[\tanh(4t) - 2\tanh(2t)] , \quad (6)$$

where $t = J/k_B T$. A mathematical relation, $e^{\alpha D} f(x) = f(x+\alpha)$ was used.

In previous papers,[7] the decoupling approximation or

$$\langle \mu_{i+\delta_1}\mu_{i+\delta_2}\mu_{i+\delta_3}\rangle \cong \langle \mu_{i+\delta_1}\rangle \langle \mu_{i+\delta_2}\rangle \langle \mu_{i+\delta_3}\rangle$$

has been used, which corresponds to the Zernike approximation in a crystalline Ising ferromagnet.[8] Instead of using the decoupling approximation, let us introduce the concept of a correlated effective field into the many-body correlation functions of neighboring spins of a particular site i;

$$\mu_{i+\delta} = \langle \mu_{i+\delta}\rangle + \lambda(\mu_i - \langle \mu_i\rangle) , \quad (7)$$

where λ is a temperature-dependent static correlation parameter.

For a ferromagnetic system with $\sigma = \langle \mu_i \rangle$, Eq. (4) reduces to, upon using the relation (7),

$$\sigma = A\sigma + B\sigma^3 \quad (8)$$

with

$$A = 4K_1 + 12K_2\lambda^2 - 8K_2\lambda^3 \quad (9)$$

and

$$B = 4K_2(1 - 3\lambda^2 + 2\lambda^3) , \quad (10)$$

from which the magnetization σ is given by

$$\sigma = \left(\frac{1-A}{B}\right)^{1/2} . \quad (11)$$

It is easily proved that magnetization σ is well defined at $T=0$, or $\sigma = 1$ at $T=0$. The transition temperature is determined from

$$1 = A(T_c) = 4K_1(T_C) + 12K_2(T_C)\lambda_c^2 - 8K_2(T_C)\lambda_c^3 . \quad (12)$$

In this way, in order to calculate the magnetization and the transition temperature within the approach, we need to evaluate the correlated-effective-field parameter λ.

For this purpose, let us use another Callen identity;

$$\langle \mu_i \mu_{i+\delta}\rangle = \langle \mu_{i+\delta} \tanh(\beta E_i)\rangle = \langle \mu_{i+\delta} e^{D\beta E_i}\rangle \tanh x|_{x=0} . \quad (13)$$

from which for a square lattice with nearest-neighbor interactions J we have

$$\langle \mu_i \mu_{i+\delta}\rangle = K_1 + K_1(\langle \mu_{i+\delta_1}\mu_{i+\delta_2}\rangle + \langle \mu_{i+\delta_1}\mu_{i+\delta_3}\rangle + \langle \mu_{i+\delta_1}\mu_{i+\delta_4}\rangle) + K_2(\langle \mu_{i+\delta_2}\mu_{i+\delta_3}\rangle + \langle \mu_{i+\delta_2}\mu_{i+\delta_4}\rangle + \langle \mu_{i+\delta_3}\mu_{i+\delta_4}\rangle) + K_2\langle \mu_{i+\delta_1}\mu_{i+\delta_2}\mu_{i+\delta_3}\mu_{i+\delta_4}\rangle . \quad (14)$$

For a ferromagnetic system, Eq. (14) reduces to, upon using relation (7) for nearest neighbors of a particular site i,

$$\sigma^2 + \lambda(1-\sigma^2) = K_1 + 3(K_1 + K_2)\sigma^2 + K_2\sigma^4 + 3(K_1 + K_2 + 2K_2\sigma^2)(1-\sigma^2)\lambda^2 - 8K_2\sigma^2(1-\sigma^2)\lambda^3 + K_2(1+3\sigma^2)(1-\sigma^2)\lambda^4 . \quad (15)$$

Thus, magnetization and the correlated-effective-field parameter can be determined by solving the coupled Eqs. (11) and (15).

Now, let us clarify how the transition temperature is elaborated in this formulation in comparison with that of Lines's method. At the Curie temperature,

Eq. (15) reduces to

$$\lambda_c = K_1(T_C) + 3[K_1(T_C) + K_2(T_C)]\lambda_c^2 + K_2(T_C)\lambda_c^4 \ . \tag{16}$$

Then, the Curie temperature T_C and the correlated-effective-field parameter at the transition point λ_c can be evaluated from Eqs. (12) and (16). For the numerical evaluation of the Curie temperature it is convenient to apply the Sylvester's determinant method to Eqs. (12) and (16).[9] We found that the T_C for the square lattice is given by

$$\frac{k_B T_C}{J} = \frac{2}{\ln 2} \ , \tag{17}$$

which is equivalent to that of the Bethe-Peierls method. Substituting the result (17) into Eq. (12), the λ_c is given by

$$\lambda_c = \tfrac{1}{3} \ . \tag{18}$$

In Fig. 1, the behavior of λ as a function of temperature is given.

In this Communication, to clarify our method we have discussed a simple case of a square Ising ferromagnetic system. The approach can be easily extended to any dimensional lattices. For example, we can easily prove that for one-dimensional Ising lattice with nearest-neighbor interactions J the transition temperature is given by $T_C = 0$. Then, the temperature-dependent correlated parameter $\lambda(T)$ is given by

$$\lambda(T) = \frac{1 - \{1 - 4[K(T)]^2\}^{1/2}}{2K(T)} \tag{19}$$

with

$$K(T) = \tfrac{1}{2}\tanh(2t) \ , \tag{20}$$

from which we can easily understand that the $\lambda(T)$ is the function of decrease from $\lambda = 1$ at $T = 0$ as temperature increases. In the same way as the square lattice, we have evaluated the T_C and λ_c for simple cubic, body-centered cubic, and face-centered-cubic ferromagnetic systems with nearest-neighbor interaction J. We found that the T_C and λ_c are given by

$$\frac{k_B T_C}{J} = \frac{2}{\ln[z/(z-2)]} \tag{21}$$

and

$$\lambda_c = \frac{1}{z-1} \ , \tag{22}$$

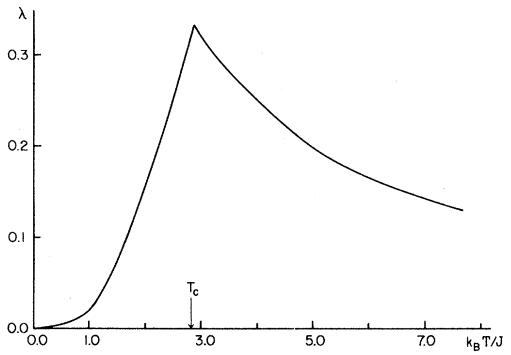

FIG. 1. Temperature dependence of λ for a square lattice.

where z is the number of nearest neighbors. The result (21) is essentially equivalent to that of the Bethe-Peierls method. It is interesting that λ_c is given by the universal function of z.

Within this method we can easily formulate the susceptibility, internal energy, and specific heat; the specific heat of a ferromagnetic lattice with nearest-neighbor interactions J is given by

$$\frac{C}{C_0} = 2t^2(1-\lambda)\sigma\frac{\partial\sigma}{\partial t} + (1-\sigma^2)t^2\frac{\partial\lambda}{\partial t} \tag{23}$$

with

$$C_0 = \frac{NZk_B}{2} \ .$$

For the one-dimensional lattice, the specific heat is given by, upon using Eq. (19),

$$\frac{C}{Nk_B} = t^2\frac{\partial\lambda}{\partial t} = \frac{2t^2\mathrm{sech}^2(2t)}{1+\mathrm{sech}(2t)} \ .$$

Finally, it is important to remark that the advantage of our method is its conceptual and mathematical simplicity. This new type of correlated-effective-field theory is expected to have wide applications for the problems in crystalline and disordered Ising magnets.[10] A detailed discussion of the method is planned to appear in a forthcoming paper.

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[10]This approach is an effective-field theory; so that it may be less sensitive than the original correlated-field theory of M. E. Lines to dimensionality criteria.