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Some Remarks on Perturbation Theory and Phase Transition with an Application to Anisotropic Ising Model

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A system with Hamiltonian H_0 is assumed to undergo a phase transition at transition temperature T_0. When a small perturbation term $\lambda H'$ is added to H_0, the transition temperature will depend on the coupling parameter λ and the critical indices will in general be changed. The change induced by the application of $\lambda H'$ is classified into three types, and these types are discussed for the cases of anisotropic Ising ferromagnets by means of thermodynamic perturbation theory and scaling law equation for spin correlation functions.

§ 1. Introduction

Suppose a system described by the Hamiltonian H_0 that undergoes a phase transition at transition temperature T_0. When a small perturbation term $\lambda H'$ is added to H_0, the feature of phase transition will be changed in some respects. Generally speaking, the order of phase transition may be altered, but let us restrict ourselves to the cases in which it is unaltered. Then one may first expect that the transition temperature T_c becomes a function of λ. As for the λ dependence of T_c, we may consider the following two possibilities: $T_c(\lambda)$ is either analytic or singular at the point $\lambda=0$. Secondly, the critical indices will be unchanged or changed according to the nature of perturbation. One may thus classify the change associated with the application of $\lambda H'$ into three types shown in the following Table.

Table I. Classification of change of phase transition.

	transition temperature	critical indices
type I	analytic in λ	no change
type II	singular in λ	no change
type III	analytic or singular in λ	change

A trivial example of type I is the case in which the perturbation Hamiltonian H' is the unperturbed one itself. That is, we change the Hamiltonian of the system from H_0 to $(1+\lambda)H_0$. It is clear that in this case the $T_c(\lambda)$ is expressed as $T_c(\lambda)=T_0(1+\lambda)$ and that the critical indices are never changed. Herman and Dorfman[1] have considered the two-dimensional Ising ferromagnet with nearest and next-nearest neighbor interactions, taking the latter interaction as perturbation.

They have shown that the qualitative feature of phase transition is essentially the same as the unperturbed one, and calculated $T_c(\lambda)$ up to the term of λ^2. Their system thus belongs to the type I by our classification.

The purpose of this paper is to discuss the types II and III, taking anisotropic Ising ferromagnets as examples. In § 2, we will consider a two-dimensional anisotropic Ising model and study the λ dependence of specific heat in the neighborhood of transition point. Some exact features of the system are emphasized, since they are taken over to a study of three-dimensional system. We will discuss in § 3 the Ising film in which a small exchange interaction is exerted between layers. By means of thermodynamic perturbation theory and scaling law equation for spin correlation functions, it is shown that the system belongs to the type II. Section 4 is devoted to a study of three-dimensional anisotropic Ising system and the λ dependences of specific heat, susceptibility, critical magnetization are discussed. A distribution of Lee-Yang zeros is also briefly referred to.

§ 2. Two-dimensional anisotropic Ising model

Consider a simple square Ising ferromagnet in which the horizontal nearest neighbor interaction is given by J and the vertical one by λJ (Fig. 1). The exact transition temperature obtained by Onsager[2] is given by the equation

$$\mathrm{sh}(2K_c)\,\mathrm{sh}(2\lambda K_c)=1\,, \tag{2·1}$$

where $K=\beta J$ ($\beta=1/kT$). When λ is positive and small, the asymptotic solution of Eq. (2·1) is found to be

$$K_c \simeq -\tfrac{1}{2}[\ln\lambda+\ln(-\tfrac{1}{2}\ln\lambda)+\cdots]. \tag{2·2}$$

Weng, Griffiths and Fisher[3] and Fisher[4] have discussed the above dependence of T_c on λ, considering a lower or an upper bound of transition temperature.

Let us now consider the present system from the following point of view. If $\lambda=0$, the vertical interaction vanishes, thus the system is reduced essentially to a one-dimensional case. Conversely, one can regard the horizontal interaction as an unperturbed Hamiltonian and the vertical one as a small perturbation. As is well known, a one-dimensional Ising system does not undergo a phase transition, but one can assume that the transition temperature in this case is absolute zero. Then one may raise a question how the feature of phase transition is modified when the perturbation $\lambda H'$ is applied. Since the main problem of this paper is

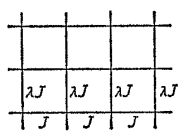

Fig. 1. Two-dimensional anisotropic Ising model.

to discuss a connection between the change of phase transition and the perturbation, it is instructive to examine the present model in some details.

The exact solution for this model obtained by Onsager[2] is

$$\frac{\ln Z}{N}=\ln 2+\frac{1}{2\pi^2}\int_0^\pi\int_0^\pi \ln(\mathrm{ch}\,2K\,\mathrm{ch}\,2\lambda K-\mathrm{sh}\,2K\cos\omega-\mathrm{sh}\,2\lambda K\cos\omega')\,d\omega d\omega', \tag{2·3}$$

where Z is the canonical partition function and N is the total number of spins. From the above equation, the specific heat near the transition point is calculated to be

$$\frac{C}{Nk}\simeq\frac{\lambda(\ln\lambda)^3}{2\pi}\ln\left|\frac{T-T_c}{T_c}\right|. \tag{2·4}$$

It is seen from Eq. (2·4) that the specific heat is divergent logarithmically for any small λ unless it is zero and that the amplitude of specific heat depends on λ. The former fact is supposed to represent a current belief that the critical indices are insensitive to details of interaction as far as it is of short-ranged. A similar situation would also be expected for a three-dimensional system, and this will be discussed in § 4. Also, our main problem will be to find the λ dependence of amplitude for some quantities of physical interest.

§ 3. Two-layer Ising film

The two-layer Ising film has been studied previously by Ballentine,[5] and more recently by Allan.[6] As a matter of fact, Allan has discussed the $n\times\infty\times\infty$ simple cubic lattices with $n=2, 3, 4$ and 5 by means of high temperature series expansion. These authors are mainly concerned with the isotropic exchange interaction, but we are going to study a two-layer problem in which the exchange interaction between layers is λJ, whereas that in a layer is J (Fig. 2). The reason for dealing with such a system is twofold: first, we would like to show that a phase transition of the system is of the type II, and secondly, the following procedure is naturally extended to a three-dimensional system. Before going into the details, we note that the present model undergoes a phase transition characteristic of a two-dimensional Ising ferromagnet,[6] in particular the susceptibility index is given by $\gamma=7/4$.

In the presence of magnetic field H, an obvious choice of unperturbed and perturbation Hamiltonian is

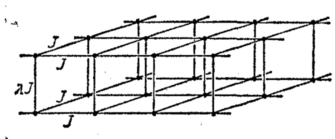

Fig. 2. Two-layer Ising film.

$$H_0=-\sum_{\text{intra layer}} Js_is_j-H\sum s_i\,, \tag{3·1a}$$

$$\lambda H'=-\sum_{\text{inter layer}} \lambda Js_is_{i'}\,. \tag{3·1b}$$

The partition function of the system is written as

$$Z=\mathrm{tr}[e^{-\beta(H_0+\lambda H')}]=\mathrm{tr}(e^{K_0+\lambda K'}), \tag{3·2}$$

where we have introduced notations $K_0=-\beta H_0$ and $K'=-\beta H'$ for simplicity. If we divide Eq. (3·2) by the partition function Z_0 for the unperturbed system, we have

$$\frac{Z}{Z_0}=\frac{\mathrm{tr}(e^{K_0}e^{\lambda K'})}{\mathrm{tr}(e^{K_0})}\equiv\langle e^{\lambda K'}\rangle\,, \tag{3·3}$$

where $\langle\ \rangle$ implies a thermodynamic average for the unperturbed system. A simple application of cumulant expansion[7] leads us to the following perturbation series:

$$\ln Z=\ln Z_0+\langle e^{\lambda K'}-1\rangle_c=\ln Z_0+\lambda\langle K'\rangle_c+(\lambda^2/2!)\langle K'^2\rangle_c+\cdots. \tag{3·4}$$

We first study the terms $\langle K'\rangle_c$ and $\langle K'^2\rangle_c$ and generalize the results to higher order terms. A quantity $\langle K'\rangle_c$ is given by

$$\langle K'\rangle_c=\langle K'\rangle=K\sum\langle s_is_{i'}\rangle\,. \tag{3·5}$$

Since there is no interaction between layers for the unperturbed Hamiltonian, we find $\langle s_is_{i'}\rangle=\langle s_i\rangle^2=\langle s\rangle^2$, thus Eq. (3·5) is reduced to

$$\langle K'\rangle_c=NK\langle s\rangle^2, \tag{3·6}$$

where N is the total number of lattice points in one layer. Next, by means of the formula of cumulant expansion, $\langle K'^2\rangle_c$ is expressed as

$$\begin{aligned}\langle K'^2\rangle_c&=\langle K'^2\rangle-\langle K'\rangle^2=K^2\sum[\langle s_is_{i'}s_js_{j'}\rangle-\langle s_is_{i'}\rangle\langle s_js_{j'}\rangle]\\&=K^2\sum_{ij}[\langle s_is_j\rangle^2-\langle s_i\rangle^2\langle s_j\rangle^2],\end{aligned} \tag{3·7}$$

where the summation by i, j is extended over lattice points on one layer (see Fig. 3).

It is unfortunately impossible to calculate Eqs. (3·6) and (3·7) exactly, but one may find some essential features of perturbation terms on the basis of scaling law. According to this law, the average $\langle s\rangle$ and the pair correlation function $g(R)$ above and near the transition point are written as[8]

$$\langle s\rangle=\varepsilon^{-\gamma+(\Delta/2)}f(h/\varepsilon^{\Delta/2}), \tag{3·8a}$$

$$g(R)=\langle s_0s_R\rangle-\langle s_0\rangle\langle s_R\rangle=\varepsilon^{\Delta-2\gamma}g(R/\xi,\,h/\varepsilon^{\Delta/2}), \tag{3·8b}$$

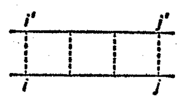

Fig. 3.

where ε is defined by

$$\varepsilon = (T - T_0)/T_0\,, \tag{3·9}$$

which describes a deviation of temperature from the unperturbed transition temperature. Furthermore, h is the magnetic field in an appropriate unit, Δ the gap parameter introduced by Domb and Hunter,[9] ξ the correlation length whose behavior in the vicinity of transition point is usually expressed as

$$\xi \propto \varepsilon^{-\nu}. \tag{3·10}$$

Since we are interested in the case of small λ, it is expected that the deviation of $T_c(\lambda)$ from T_0 is small, so that we may assume that $\varepsilon \ll 1$. Therefore, the scaling law equations valid for small ε are applicable for the following discussions.

Combining Eq. (3·6) with Eq. (3·8a), we have

$$\langle K' \rangle_c = N\varepsilon^{\Delta - 2\gamma} \psi_1 (h/\varepsilon^{\Delta/2}), \tag{3·11}$$

where a quantity K is included in the definition of ψ_1. Furthermore, from Eqs. (3·7) and (3·8b), it follows that

$$\langle K'^2 \rangle_c = K^2 N \sum_R g(R) \{\langle s_0 s_R \rangle + \langle s_0 \rangle \langle s_R \rangle\}. \tag{3·12}$$

Since a main contribution to the sum comes from a region with large R, one may replace the sum by an integral and approximate a quantity in curly brackets by $2\langle s \rangle^2$. As a result, we get

$$\langle K'^2 \rangle_c \propto N \int_0^\infty \varepsilon^{2\Delta - 4\gamma} g\left(\frac{R}{\xi}, \frac{h}{\varepsilon^{\Delta/2}}\right) f^2\left(\frac{h}{\varepsilon^{\Delta/2}}\right) R dR\,.$$

Introducing a change of variable $R = \xi t$ and using a scaling law relation $\nu d = \Delta - \gamma$ with d the dimensionality ($d=2$ in the present case), we find

$$\langle K'^2 \rangle_c = N\varepsilon^{\Delta - 3\gamma} \psi_2 (h/\varepsilon^{\Delta/2}). \tag{3·13}$$

The above procedure is easily extended to higher order terms of perturbation series. In general, a term $\langle K'^n \rangle_c$ is expressed by means of n-body spin correlation function. A generalization of scaling law to this function was discussed by Kawasaki,[10] and an application of his results yields

$$\langle K'^n \rangle_c = N\varepsilon^{\Delta - (n+1)\gamma} \psi_n (h/\varepsilon^{\Delta/2}). \tag{3·14}$$

In this way, the perturbation series (3·4) is shown to be expressed as

$$\ln Z = \ln Z_0 + N \sum_{n=1}^\infty \lambda^n \varepsilon^{\Delta - (n+1)\gamma} \varphi_n \left(\frac{h}{\varepsilon^{\Delta/2}}\right). \tag{3·15}$$

Furthermore, a scaling law equation for $\ln Z_0$ reads

$$\ln Z_0 = N\varepsilon^{\Delta - \gamma} \varphi_0 (h/\varepsilon^{\Delta/2}). \tag{3·16}$$

Therefore, combining Eqs. (3·15) and (3·16), we have

$$\ln Z = N\sum_{n=0}^{\infty}\lambda^n \varepsilon^{\Delta-(n+1)\gamma}\varphi_n\left(\frac{h}{\varepsilon^{\Delta/2}}\right). \qquad (3\cdot17)$$

It is recognized from this equation that higher order terms are more divergent in the limit $\varepsilon\to0$. However, since Eq. (3·17) is essentially a power series in terms of $\lambda/\varepsilon^\gamma$, one can write Eq. (3·17) in the following form:

$$\ln Z/N = \varepsilon^{\Delta-\gamma}\Phi_2(\lambda/\varepsilon^\gamma, h/\varepsilon^{\Delta/2}). \qquad (3\cdot18)$$

This equation implies that the coupling parameter λ is scaled as a factor $\lambda/\varepsilon^\gamma$. Therefore, Eq. (3·18) may be regarded as a generalization of usual scaling law to the case where the perturbation Hamiltonian is applied.

We are now going to discuss a shift of transition temperature. To do this, we set $h=0$ and remember that the present model should exhibit a phase transition which is characteristic of two-dimensional system. This means that the behavior of $\ln Z/N$ in the vicinity of $T_c(\lambda)$ and above the transition point is expressed as

$$\ln Z/N = C\varepsilon'^{\Delta-\gamma}, \qquad (3\cdot19)$$

where C is a constant and ε' is given by

$$\varepsilon' = [T - T_c(\lambda)]/T_c(\lambda). \qquad (3\cdot20)$$

On the other hand, putting $h=0$ in Eq. (3·18), we find

$$\ln Z/N = \varepsilon^{\Delta-\gamma}\Phi_2(\lambda/\varepsilon^\gamma, 0). \qquad (3\cdot21)$$

Thus, equating Eqs. (3·19) and (3·21), we get

$$\varepsilon' = \varepsilon F(\lambda/\varepsilon^\gamma). \qquad (3\cdot22)$$

Just at the transition temperature $T_c(\lambda)$, the quantity ε' should be zero. Since the transition temperature is expected to increase as an application of perturbation, ε is positive at $T_c(\lambda)$. Consequently, in order to satisfy Eq. (3·22), a function $F(x)$ should have a zero point which we denote as $1/A^\gamma$. As a result, we have at $T=T_c(\lambda)$ that $\varepsilon = A\lambda^{1/\gamma}$ or $[T_c(\lambda)-T_0]/T_0 = A\lambda^{1/\gamma}$. From this relation, it follows that

$$T_c(\lambda) = T_0(1 + A\lambda^{1/\gamma}). \qquad (3\cdot23)$$

Since $\gamma=7/4$, $T_c(\lambda)$ has a branch point at $\lambda=0$. Therefore, we can conclude that the present model belongs to the type II according to our classification.

§ 4. Three-dimensional anisotropic Ising model

If one increases the number of layers of Ising film discussed in § 3 from 2, 3, ⋯ to ∞, one may have a three-dimensional anisotropic system. This system is expected to undergo a phase transition characteristic of three dimension irrespectively of λ unless λ is zero, in the same sense that a two-dimensional anisotropic system behaves two-dimensionally as far as $\lambda \neq 0$. Therefore, the phase transition of the present model will be described by three-dimensional critical indices.

As in § 3, it is natural to take an assembly of independent two-dimensional layers as unperturbed Hamiltonian and the interaction between layers as perturbation. Then, as mentioned above, one would expect that an application of perturbation changes the critical indices from two-dimensional ones to three-dimensional ones, however small the perturbation may be. In other words, the present model belongs to the type III.

Perturbation expansion for the system under consideration is carried out in the same way as in § 3. For instance, a term $\langle K'^2 \rangle_c$ is given by

$$\langle K'^2 \rangle_c = K^2 \sum_{ij} [\langle s_i s_{i'} s_j s_{j'} \rangle - \langle s_i s_{i'} \rangle \langle s_j s_{j'} \rangle].$$

This expression is formally identical to Eq. (3·7), but we have to note that the sum extends over all the lattice points. It is easily seen that a contribution of configuration shown by Fig. 4 vanishes; remaining terms come from the configurations indicated by (a) and (b) in Fig. 5. Applying scaling law equations and repeating the same procedure as in the previous section, we get essentially the same result as Eq. (3·13). In connection with this, we would like to note that Nesis[11] has already obtained a similar result.

A generalization of the above procedure to higher order terms can be performed as in § 3. Then it turns out that a contribution of the n-th order term is essentially the same as Eq. (3·14). Thus, the $\ln Z$ per lattice point is expressed as

$$\ln Z/N = \varepsilon^{\Delta-\gamma} \Phi_3 (\lambda/\varepsilon^{\gamma}, h/\varepsilon^{\Delta/2}). \tag{4·1}$$

Since the system is expected to behave three-dimensionally, the behavior of $\ln Z/N$ for $h=0$ has a form

$$\ln Z/N \propto \varepsilon'^{\Delta'-\gamma'}, \tag{4·2}$$

where ε' is defined by Eq. (3·20), Δ' and γ' are critical indices for a three-dimensional Ising ferromagnet. Hereafter, we will denote the quantities of three dimension by putting primes.

On the basis of Eqs. (4·1) and (4·2), a shift of transition temperature is found in the same way as in § 3. We are led to

$$T_c(\lambda) = T_0 (1 + B\lambda^{1/\gamma}). \tag{4·3}$$

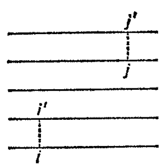

Fig. 4.

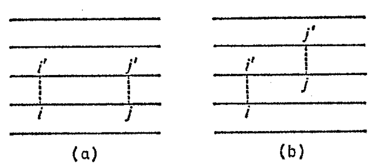

Fig. 5.

It is convenient for further discussions to transform from ε to ε'. Eliminating T from the defining equations for ε and ε' and using Eq. (4·3), we find

$$\varepsilon=\varepsilon'+B\lambda^{1/\gamma}. \tag{4·4}$$

Substituting Eq. (4·4) into Eq. (4·1), and choosing $\lambda/\varepsilon'^{\gamma}$ as a new variable, we have

$$\ln Z/N \equiv f_3(\lambda,\varepsilon',h)=\varepsilon'^{\Delta-\gamma}\Psi(\lambda/\varepsilon'^{\gamma},h/\varepsilon'^{\Delta/2}). \tag{4·5}$$

We are now in a position to discuss λ dependences of amplitudes of physical quantities such as specific heat, susceptibility, etc. By putting $h=0$ in Eq. (4·5) and noting Eq. (4·2), we get

$$f_3(\lambda,\varepsilon')\propto\varepsilon'^{\Delta'-\gamma'}=\varepsilon'^{\Delta-\gamma}\Psi(\lambda/\varepsilon'^{\gamma}). \tag{4·6}$$

The middle equation on the above line should be valid for $\varepsilon'\ll1$, so should be the right-hand side. Keeping λ fixed, taking the limit $\varepsilon'\to0$ and assuming that $\Psi(x)\sim x^p$ for $x\to\infty$, we have

$$p=[\Delta-\gamma-(\Delta'-\gamma')]/\gamma\,. \tag{4·7}$$

Or, using a scaling law relation $\Delta-\gamma=2-\alpha$, $\Delta'-\gamma'=2-\alpha'$ with α and α' are critical indices for specific heat for two and three dimensions, respectively, we find

$$p=(\alpha'-\alpha)/\gamma\,. \tag{4·8}$$

In this way, the λ dependence of free energy in the absence of magnetic field is expressed as

$$f_3(\lambda,\varepsilon')\propto\lambda^{(\alpha'-\alpha)/\gamma}\varepsilon'^{\Delta'-\gamma'},$$

and therefore that of specific heat is given by

$$C\propto\lambda^{(\alpha'-\alpha)/\gamma}\varepsilon'^{-\alpha'}. \tag{4·9}$$

A numerical result[9] $\alpha'=1/8$ and rigorous results $\alpha=0$, $\gamma=7/4$ lead us to $C\propto\lambda^{1/14}\varepsilon'^{-1/8}$. In the same way, the λ dependence of susceptibility is shown to be

$$\chi\propto\lambda^{(\gamma'-\gamma)/\gamma}\varepsilon'^{-\gamma'}, \tag{4·10}$$

whence it follows that $\chi\propto\lambda^{-2/7}\varepsilon'^{-5/4}$ by the use of a result $\gamma'=5/4$.

The above procedure is easily extended to a discussion of critical behavior of magnetization at $\varepsilon'=0$. From Eq. (4·5), the magnetization M is generally expressed as

$$M=\varepsilon'^{(\Delta/2)-\gamma}\Phi(\lambda/\varepsilon'^{\gamma},h/\varepsilon'^{\Delta/2}). \tag{4·11}$$

Assuming that $M\propto h^{1/\delta'}$ and $\Phi(x,y)$ behaves as $\Phi(x,y)\sim x^py^q$ for $x,y\to\infty$, we find putting $\varepsilon'=0$

$$q=1/\delta', \qquad (\Delta/2)-\gamma-p\gamma-q(\Delta/2)=0. \tag{4·12}$$

By the use of a scaling law relation $1/\delta=(\Delta-2\gamma)/\Delta$, we have from Eq. (4·12) $p=(\Delta/2\gamma)(\delta^{-1}-\delta'^{-1})$. Thus we are led to

$$M \propto \lambda^{(\Delta/2\gamma)(\delta^{-1}-\delta'^{-1})} h^{1/\delta'}. \tag{4·13}$$

Substitution of numerical values results in $M \propto \lambda^{-2/7} h^{1/5}$.

Equations (4·9), (4·10) and (4·13) are considered as a generalization of Eq. (2·4). It is an interesting aspect of the λ dependence that the power of λ is expressed as a mixture of two-dimensional critical indices and three-dimensional ones. In connection with this, it should be noticed that the critical indices are independent of dimensionality in a classical theory of phase transition, so that the amplitudes of physical quantities become λ independent in this theory. In other words, the fact that the amplitudes do depend on λ is regarded as a deviation of true phase transition from a prediction of classical theory.

In closing this paper, we would like to add one remark on a distribution on Lee-Yang[12] zeros in the present case. By repeating the same discussion as in a previous paper[13] and using Eq. (4·10), we can find that the λ dependence of critical angle θ_c is given by

$$\theta_c \propto \lambda^{(\Delta-\Delta')/2\gamma} \varepsilon'^{\Delta'/2}. \tag{4·14}$$

The results[9] $\Delta = 15/4$ and $\Delta' = 25/8$ give rise to the dependence $\theta_c \propto \lambda^{5/28} \varepsilon'^{25/16}$. The distribution of Lee-Yang zeros was examined for an isotropic finite system by computer calculation.[14] It would be of considerable interest to extend a similar calculation to an anisotropic system.

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