EFFECT OF SMALL PERTURBATIONS ON THE SHIFT OF THE CRITICAL POINT OF A SECOND-ORDER PHASE TRANSITION

M. A. MIKULINSKIĬ

All-union Institute of Physico-technical and Radio-engineering Measurements

Submitted September 4, 1970; resubmitted October 29, 1970

Zh. Eksp. Teor. Fiz. 60, 1445–1451 (April, 1971)

By using the assumptions of scaling theory for second-order phase transitions a method is developed for calculating the shift in the critical temperature in the system due to a superposition of small perturbations. The dependence (on the magnitude of the small perturbation) of the coefficients of the power functions in the specific heat, the magnetic moment and the susceptibility is estimated. Two examples are considered. In the first, the unperturbed system is an Ising model of arbitrary dimensions with nearest-neighbor interaction between the spins. The perturbation is the interaction along the diagonals (ϵ is the magnitude of this interaction). The temperature shift is proportional to ϵ. In the second example an arbitrary number of planes of spins arranged on top of each other are considered. The perturbation is the small interaction ($\sim\epsilon$) between the planes. The temperature shift is proportional to $\epsilon^{4/7}$.

1. INTRODUCTION

WIDOM,[1] Patashinskiĭ and Pokrovskiĭ[2] and Kadanoff[3] have developed a theory of second-order phase transitions based on dimensional estimates. This theory leads to the result that all the critical indices can be expressed in terms of two independent parameters. In this paper this method is used to solve a particular group of problems.

For definiteness, we consider the Ising model, in which the energy E of the system consists of two parts

$$E = E_0 + E_1, \tag{1}$$

where

$$E_0 = -J\sum \sigma_i\sigma_j,$$

J is the exchange energy, $\sigma_i = \pm 1$ is the spin variable, and i is the label of the lattice site at which the given spin is positioned;

$$E_1 = -\varepsilon \sum_{i_1 \ldots i_n} \sigma_{i_1}\sigma_{i_2}\ldots\sigma_{i_n} = -\varepsilon\sum_j E_j \quad (n = 1, 2, \ldots),$$

E_1 is the perturbation applied to the system, ϵ is a small parameter ($\epsilon \ll J$), $E_j = \sigma_{i_1}, \ldots \sigma_{i_n}$, and the index j includes the totality of coordinates $i_1, \ldots, i_n$. The summation in E_1 is carried out according to given rules. For the characteristic distances between the spins appearing in E_1 we take the interatomic spacings.

The difficulty of constructing the perturbation theory is due to the fact that the partition function in the zeroth approximation in ϵ at the transition point T_0 of the unperturbed system is not analytic, and so the expansion of the partition function Z in a Taylor series is performed not in the parameter ϵ but in the parameter ϵ/τ_0^c ($\tau_0 = (T - T_0)/T_0$, T is the temperature of the system, and c is a constant). Summing all the terms of the series leads to the result that Z can be expressed in terms of an unknown function of one parameter $\xi = \epsilon/\tau_0^c$, and this makes it possible to obtain certain qualitative relations between the parameters of the theory.

The perturbation E_1 can lead to two different cases: 1) the phase transition in the system disappears (an example is the application of an external magnetic field to a ferromagnet), 2) the phase transition does not disappear, but there is a shift in the critical point. In the paper we examine in detail an example of the second case: an Ising model consisting of an arbitrary number of planes arranged on top of each other, with weak interaction between them. We succeed in finding the dependence of the shift of the critical point on the parameter ϵ of the interaction between the planes ($\Delta T \propto \epsilon^{4/7}$). We also find the dependence on ϵ of the specific heat, the magnetic moment and the susceptibility.

2. GENERAL METHOD

The partition function corresponding to the energy (1) has the form

$$Z = \sum_{\{\sigma\}} \exp\left(-\frac{E_0}{T}\right)\exp\left(\Theta\sum_j E_j\right), \tag{2}$$

where T is the temperature of the system and $\Theta = \epsilon/T$; the summation in (2) is performed over all spin configurations.

It is easy to verify the identity

$$\exp(\Theta E_j) \equiv \operatorname{ch}\Theta(1 + zE_j), \quad z = \operatorname{th}\Theta, \tag{3}$$

and using this we rewrite (2) in the form

$$Z = \operatorname{ch}^{Nh}\Theta \cdot \sum_{\{\sigma\}} e^{-E_0/T}\prod_j (1 + zE_j)$$

$$= \operatorname{ch}^{Nh}\Theta \cdot Z_0 \sum_{p=0}^{\infty} z^p \sum_j \langle E_{j_1}E_{j_2}\ldots E_{j_p}\rangle. \tag{4}$$

Here h is a constant depending on the rules for summing over i in E_1, N is the number of sites in the system, $Z_0 = \sum \exp(-E_0/T)$,

$$\langle E_{j_1}\ldots E_{j_p}\rangle = \sum E_{j_1}\ldots E_{j_p} e^{-E_0/T}/Z_0$$

is the correlator p of the energies (1), each of which is in the form of a product of n spins. The correlators of the unperturbed system appear in (4).

By using the method proposed by Patashinskiĭ and Pokrovskiĭ,[2] we introduce the irreducible correlators Q by the formulas

$$Q(j)=\langle E_j\rangle,\quad Q(j_1,j_2)=\langle E_{j_1}E_{j_2}\rangle-Q(j_1)Q(j_2),$$
$$Q(j_1,j_2,j_3)=\langle E_{j_1}E_{j_2}E_{j_3}\rangle-Q(j_1)Q(j_2,j_3)-$$
$$-Q(j_2)Q(j_1,j_3)-Q(j_3)Q(j_1,j_2)-Q(j_1)Q(j_2)Q(j_3),\ldots \tag{5}$$

The correlators Q go to zero if any distances between the spins appearing in Q are greater than the correlation range $\sim r_0$ of the unperturbed sytem.

The inverse relations have the form

$$\langle E_j\rangle=Q(j),\quad \langle E_{j_1}E_{j_2}\rangle=Q(j_1,j_2)+Q(j_1)Q(j_2),$$
$$\langle E_{j_1}E_{j_2}E_{j_3}\rangle=Q(j_1,j_2,j_3)+Q(j_1)Q(j_2j_3)$$
$$+Q(j_2)Q(j_1,j_3)+Q(j_3)Q(j_1,j_2)+Q(j_1)Q(j_2)Q(j_3),\ldots \tag{6}$$

Putting (6) into (4) and using a theorem from [4] (Sec. 15) which enables us to express the free energy F in terms of the irreducible correlators only, we obtain

$$F=F_r+F_0+\sum_{p=1}^{\infty}z^p\sum_j Q(j_1,\ldots,j_p), \tag{7}$$

where F_r is the regular part of the free energy and F_0 is the free energy of the unperturbed system.

We shall consider the case when the perturbation E_1 leads to a shift in the critical temperature. In this case E_j consists of a product of an even number of spins.

We shall estimate the correlators occurring in (7) by the method of scaling theory.[3] The Kadanoff transformation from microscopic quantities to cell quantities (with cell dimensions $\bar{L}$) has the form

$$r\to r/\bar{L},\quad \tau_0\to\tau_0\bar{L}^{y_0},\quad E_1\to E_1\bar{L}^{-a}, \tag{8}$$

where y_0 and a are critical indices in the unperturbed system; the constant a depends on the number of spins and on the rules for the summation in E_1 and in every concrete case can be expressed in terms of the indices x_0 and y_0.

For the estimates we can assume that all distances between spins in the correlator are the same order: $r\sim r_0$. Then

$$Q_p(r,\tau_0)=Q(j_1\ldots j_p)\sim\langle E_{j_1}\ldots E_{j_p}\rangle=\bar{L}^{-pa}\langle\bar{E}_{j_1}\ldots\bar{E}_{j_p}\rangle$$
$$=\bar{L}^{-pa}Q_p(r/\bar{L},\tau_0\bar{L}^{y_0}).$$

The general solution satisfying this equation is

$$Q_p(r,\tau_0)=\tau_0^{pa/y_0}Q_p(r\tau_0^{1/y_0}). \tag{9}$$

In the limiting case $r\tau_0^{1/y_0}\ll 1$ (or $r\ll r_0$) we have

$$Q_p(r,\tau_0)\sim r^{-pa}. \tag{10}$$

Using the formula (10), we obtain a dimensional estimate for Γ_p:

$$\Gamma_p=\sum_j Q(j_1\ldots j_p)\sim\frac{Nr_0^{d(p-1)}}{r_0^{pa}}\sim Nr_0^{-d}r_0^{p(d-a)}\sim$$
$$\sim N\tau_0^{d/y_0}\tau_0^{-p(d-a)/y_0}, \tag{11}$$

where d is the dimensionality of the space.

Putting (11) into (7), we rewrite the expression for the singular part F_s of the free energy in the form

$$F_s=N\tau_0^{d/y_0}\sum_{p=1}^{\infty}b_p\left(\frac{z}{\tau_0^{(d-a)/y_0}}\right)^p=N\tau_0^{d/y_0}f(\xi), \tag{12}$$

where the b_p are constants and $\xi=z/\tau_0^{(d-a)/y_0}$.

At the phase transition point $f(\xi)$ has a singularity, i.e., there exists a point ξ_0 at which the function $f(\xi)$ is nonanalytic. There are no parameters at our disposal from which it would be possible to construct small (or large) numbers, and therefore $\xi_0\sim 1$.

From (12) follows an equation for the transition temperature T_c of the system under consideration:

$$\xi_0=z/\tau_{0c}^{(d-a)/y_0},\quad \tau_{0c}=(T_c-T_0)/T_0. \tag{13}$$

From (13) we have the desired formula, determining the dependence of T_c on z:

$$T_c=T_0\left(1+\left(\frac{z}{\xi_0}\right)^{y_0/(d-a)}\right), \tag{14}$$

i.e., the shift in the transition temperature on application of the perturbation is proportional to ϵ exp $y_0/(d-a)$.

We shall examine the regions $\xi\ll 1$ ($z\ll\tau_0^{(d-a)/y_0}$) and $\xi\gg 1$ ($z\gg\tau_0^{(d-a)/y_0}$). In the first region ($z\to 0$), expression (12) for F_s must go over to $F_{s0}\sim N/r_0^d$, the free energy of the unperturbed problem, i.e., $f(\xi)\to$ const as $\xi\to 0$. In the second region ($z\gg\tau_0^{(d-a)/y_0}$, $\tau_0\to 0$), the singular part of the specific heat C has the behavior

$$C\sim N\tau_0^{-\alpha_0}f_1(\xi),\quad \alpha_0=2-d/y_0. \tag{15}$$

In this region, the specific heat should not have a singularity, i.e., C should not depend on τ_0, whence

$$C\sim z^{-\alpha_0y_0/(d-a)}\sim\varepsilon^{-(2y_0-d)/(d-a)}. \tag{16}$$

By using formula (14) in the expression (12) for the free energy, it is easy to go over from the variable τ_0 to the variable $\tau=(T-T_c)/T_0$:

$$F=F_r+N\tau_0^{2-\alpha_0}Tf_2(\eta); \tag{17}$$

here, f_2 is a new unknown function of the parameter $\eta=z/\tau$ exp $(d-a)/y_0$.

We shall determine the dependence of ϵ of the coefficients of the power functions of τ in the specific heat, the magnetic moment M and the susceptibility χ. In the region $\tau\gg z$ exp $y_0/(d-a)$ ($z\to 0$), these thermodynamic variables must behave like the solutions of the unperturbed problem:

$$C\sim\tau^{-\alpha_0},\quad M\sim\tau^{\beta_0},\quad \chi\sim\tau^{-\gamma_0}. \tag{18}$$

In the region $\tau\ll z$ exp $y_0/(d-a)$ let them be described by the formulas

$$C\sim\varepsilon^{\alpha_1}\tau^{-\alpha},\quad M\sim\varepsilon^{\beta_1}\tau^{\beta},\quad \chi\sim\varepsilon^{\gamma_1}\tau^{-\gamma}, \tag{19}$$

(Between the exponents α, β, and γ there exists the usual scaling theory relation $\alpha+2\beta+\gamma=2$.) It is easiest to find the exponents α_1, β_1, and γ_1 by "matching" the formulas (18) and (19) in the region $\tau\sim\epsilon\times$ exp $y_0/(d-a)$, whence we obtain the desired formulas

$$\alpha_1=\frac{(y-y_0)d}{y(d-a)},\quad \beta_1=\frac{dy-yx_0-dy_0+y_0x}{y(d-a)},$$
$$\gamma_1=\frac{yd-2x_0y-dy_0+2xy_0}{y(d-a)}. \tag{20}$$

Here x_0, y_0 and x, y are the Kadanoff transformation exponents in the unperturbed and perturbed systems respectively.

To conclude this section, we note one important fact. At the true transition point r_0 is finite, and in the approximation (10) and (11), we have a system of finite non-interacting regions of dimensions $\sim r_0$. In such a system, the phase transition is "blurred". Nevertheless, the use of the method presented above is justified, since the temperature interval of the "blurring" $\overline{\tau}$ is less than or of the order of the shift τ_{0C} in the transition temperature. In fact, the phase transition is "blurred" in the temperature region in which the true correlation range of the system $r_C \sim 1/(\overline{\tau} \exp 1/y)$ becomes of the order of or greater than the dimensions of the non-interacting regions $r_0 \sim 1/\tau_0^{1/y_0} \gtrsim \tau_{0C}^{-1/y_0}$, whence we obtain a limit for the blurring temperature $\overline{\tau} \lesssim \tau_{0C}^{y/y_0}$. It is easy to show that if the specific heat index α does not decrease as a result of applying the perturbation, then $y/y_0 \geq 1$, i.e., $\overline{\tau} \lesssim \tau_{0C}$.

We shall examine the Ising model with nearest-neighbor interaction in the zeroth approximation. As E_1 we introduce an Ising interaction along the diagonals. Then E_1 transforms in (8) as an energy, $a = d - y_0$, and from (14) we obtain $\tau_{0C} \sim \epsilon$. In the two-dimensional Ising model, this result is in agreement with the exact formulas obtained in [5].

3. AN ISING MODEL CONSISTING OF AN ARBITRARY NUMBER OF INTERACTING SPIN PLANES

We shall consider a system consisting of two interacting spin planes, one on top of the other. The energy of such a system has the form

$$E = E_0 - \varepsilon \sum_{k,l} \sigma_{kl1}\sigma_{kl2}. \tag{21}$$

Here E_0 is the interaction energy of the spins within the Ising planes, ϵ is the interaction constant of the spins positioned in different planes, and the index i labels the planes.

In this case the zeroth-approximation partition function breaks down into a product of partition functions referring to the first and second planes, and in formula (7) the spins belonging to different planes are averaged independently. Therefore, E_j transforms in the Kadanoff transformations as the square of the magnetic moment, i.e., $E_1 \to L \exp[2(x_0 - d)] \times \overline{E}_1$, whence $a = 2(d - x_0) = 1/4$. Putting this value of a into (14), we obtain the desired formula

$$T_c = T_0(1 + (z/\xi_0)^{4/7}). \tag{22}$$

This result can also be obtained directly from (7), taking account of the independent averaging of the spins in different planes and estimating Q from the formula

$$\sum_j Q(j_1 \ldots j_{2p}) \sim \sum_j \langle \sigma_{j_1} \ldots \sigma_{j_{2p}} \rangle^2 \sim r_0^{4p} \langle \sigma_1 \sigma_{1+r_0} \rangle^{2n} \sim \tau_0^{-7n/2}.$$

This estimate of the correlator and also the estimates (10) and (11) have been confirmed by exact calculations in the framework of the two-dimensional Ising model.[6]

Thus, the shift in the critical temperature is proportional to $\epsilon^{4/7}$.

We now consider an Ising lattice consisting of L interacting planes. The energy of such a system has the form

$$E = E_0 - \varepsilon \sum_{k,l,m} \sigma_{klm}\sigma_{klm+1}, \tag{23}$$

where the indices k and l characterize the position of the spins within the two-dimensional planes and the index m labels the planes. In this case, for not too large L the formula (22) is conserved, with ξ_0 depending on L. If, however, the number of planes is large enough, the corrections to the multiplicative estimates of the correlators can, being multiplied by L, become greater than the basic terms. In this case we cannot prove (22). To calculate the range of L in which expression (22) is applicable, we use the following method (pointed out by A. M. Polyakov). We calculate the quantity $\partial M/\partial z$ as $z \to 0$ from the formula

$$\frac{\partial M(\tau_0, z=0)}{\partial z} = \frac{\partial}{\partial z}\left\langle \sigma_{001} \exp\left(\Theta \sum_{k,l,m} \sigma_{klm}\sigma_{klm+1}\right)\right\rangle\Big|_{z=0} \tag{24}$$

(the symbol $\langle\ \rangle$ denotes averaging with weight $\exp(E_0/T)$).

Taking into account that averaging of spins belonging to different planes is independent, from (24) we obtain

$$\frac{\partial M(\tau_0, z=0)}{\partial z} = \chi_0 M_0 + (L-2)M_0^3 \sim \tau_0^{-7/4}\tau_0^{1/8} + (L-2)\tau_0^{3/8}. \tag{25}$$

We obtain from (25) that $M(z, \tau_0)$ as $z \to 0$ has the form $\tau_0^{1/8} f(z/\tau_0^{7/4})$ only in the case when the first term of the right-hand side of (25) is much greater than the second. By comparing them we find the region of applicability of (22) in L: $L - 2 \ll \tau_0^{-1}$. This condition must be fulfilled in the whole range of temperatures from T_0 to T_C.

Assuming that in the region $\tau \ll \epsilon^{4/7}$ the specific heat, magnetic moment and susceptibility are described by the equalities (19), by "matching" the formulas in the regions $\tau \ll \epsilon^{4/7}$ and $\tau \gg \epsilon^{4/7}$ we obtain

$$\alpha_1 = {}^4/_7\alpha, \quad \beta_1 = {}^1/_{14} - {}^4/_7\beta, \quad \gamma_1 = {}^4/_7\gamma - 1. \tag{26}$$

The formulas obtained can be verified experimentally in layer-structure films of the type $CoCl_2$, $FeBr_2$, NiI_2, etc. by changing ϵ by applying an external pressure P to the samples and assuming that these substances can be described by the Ising model. (In the Heisenberg model, two dimensional structures do not have a phase transition.) It is natural to assume that at small pressures

$$\varepsilon = \varepsilon_0 + BP, \tag{27}$$

where ϵ_0 is the value of the exchange integral at $P = 0$ and B is a constant. Putting (27) into (22), we obtain the pressure dependence of the transition temperature. The formulas (22) and (26) can also be verified by direct computer calculations.

The formulas (14) and (20), obtained for the Ising model, can easily be generalized to other systems. In fact, the free energy of any system can be expressed in terms of a sum of connected diagrams ([4], Sec. 15); this is the generalization of formula (7). The n-th order connected diagrams can be estimated from the formula (11), and this leads to the expressions (14) and (20).

In conclusion, the author thanks M. Sh. Giterman, A. I. Larkin, V. L. Pokrovskiĭ and A. M. Polyakov for useful discussions.

[1] B. Widom, J. Chem. Phys. **43**, 3892 (1965).
[2] A. Z. Patashinskiĭ and V. L. Pokrovskiĭ, Zh. Eksp. Teor. Fiz. **50**, 439 (1966) [Sov. Phys.-JETP **23**, 292 (1966)].
[3] L. P. Kadanoff, Physics **2**, 263 (1966).
[4] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Metody kvantovoĭ teorii polya v statisticheskoĭ fizike (Quantum Field Theoretical Methods in Statistical Physics) Fizmatgiz, 1962 [English Transl., Pergamon Press, Oxford, 1965].
[5] V. G. Vaks, A. I. Larkin, and Yu. A. Ovchinnikov, Zh. Eksp. Teor. Fiz. **49**, 1180 (1965) [Sov. Phys.-JETP **22**, 820 (1966)].
[6] M. A. Mikulinskiĭ, Zh. Eksp. Teor. Fiz. **58**, 1848 (1970) [Sov. Phys.-JETP **31**, 991 (1970)].

Translated by P. J. Shepherd
159