Isomorphism of Phase Transitions

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We analyze the conservation of the type of singularity of thermodynamic quantities near a second-order phase transition point when a small perturbation is turned on. It is shown that if the temperature shift is a non-analytic function of the magnitude of the perturbation, then the singularities of the perturbed and unperturbed systems have different forms. The Ising model corresponding to two interacting planes and the Ising model with nearest-neighbor interaction J_0 and with interaction along the diagonals J_1 (in the case when $J_0/J_1 \ll 1$) cannot have a logarithmic singularity in the specific heat with a pre-logarithmic coefficient that is analytic in J_0 and in the temperature. In the opposite limiting case $J_0/J_1 \gg 1$ and in the principal approximation in this parameter, the Ising model with interaction along the diagonal has a logarithmic singularity. The influence of equilibrium impurities on the thermodynamics of the phase transition of a ferromagnet is considered. It is shown that the Syozi model with allowance for direct interaction between the impurities is equivalent, in the principal approximation with respect to this interaction, to an Ising model without impurities but with interaction along the diagonals.

At present there is a small number of exactly-solved models of phase transitions[1-3]. When these models are made more complicated by including perturbations (e.g., interactions along the diagonals in the two-dimensional Ising model), it becomes impossible in most cases to obtain an exact solution. We propose here a method that makes it possible to establish whether the singularities of the thermodynamic quantities remain unchanged when a weak perturbation is turned on. If the singularities of the thermodynamic quantities with respect to temperature do not change when the perturbation is turned on, and the coefficient of the singularity is an analytic function of the temperature and of the magnitude of the perturbation (only a shift of the critical point takes place), we shall call this isomorphism of the phase transition in the perturbed and unperturbed systems. The unperturbed system will henceforth be regarded as an Ising model with nearest neighbor interaction.

We shall prove that there is no isomorphism if the shift of the critical point is not analytic in the perturbation. Let us assume the contrary, that there is isomorphism. Then the singular part of the free energy F_S can be written in the form

$$F_s = C(T, \varepsilon)\tau^{2-\alpha_0}, \tag{1}$$

where T is the temperature, ϵ the perturbation parameter, $C(T, \epsilon)$ an analytic function of T and ϵ, $\tau = (T - T_c)/T_0$, T_c and T_0 are the critical temperatures of the perturbed and unperturbed systems, respectively, and α_0 is the critical exponent in the unperturbed system.

Let the shift of the critical temperature be

$$(T_c - T_0)/T_0 = \tilde{A}\varepsilon^d, \tag{2}$$

where $\tilde{A}$ is a constant (~ 1) and d is by assumption a non-integer number.

Substituting (2) in (1), we obtain the following expression for F_S:

$$F_s = C(T, \varepsilon)(\tau_0 - \tilde{A}\varepsilon^d)^{2-\alpha_0}, \tag{3}$$

where $\tau_0 = (T - T_0)/T_0$.

It was shown earlier[4] that the singular part of the free energy can be represented in the form of a series in integer powers of $\epsilon/\tau_0^{1/d}$, which converges in the region $\epsilon/\tau_0^{1/d} \ll 1$, since the free energy has no singularities as $T \to \infty$. Obviously, the expression (3) cannot be represented in the form of this series, since it is a non-analytic function of ϵ as $\epsilon \to 0$.

Thus, our assumption that the representation (1) is valid where F_S is not satisfied, and the system with the perturbation is not isomorphic to the unperturbed system.

In the first section of this paper we investigate the analytic properties of the coefficient $C(T, \epsilon)$. In subsequent sections we consider examples in which turning on the perturbation leads both to violation and to conservation of the isomorphism.

In the second section we consider two interacting spin planes located one over the other, and the Ising model with interaction along the diagonals in the case when the ratio of the constant of the interaction along the diagonals J_1 and between the nearest neighbors J_0 satisfies the inequality $J_1/J_0 \gg 1$. In these systems, the isomorphism is violated.

In the third section, the Ising model with interaction along the diagonals is considered in the opposite limiting case $J_1/J_0 \ll 1$. It is shown that in the principal approximation in the parameter J_1/J_0 this model is isomorphic to the Ising model with nearest-neighbor interaction.

It is shown in the fourth section that the Syozi model[3] with allowance for the direct interaction between the impurities is isomorphic in the principal approximation in the concentration to the Ising model with interaction along the diagonals.

1. We apply to a certain system a perturbation of magnitude ϵ. The ensuing shift of the critical point is described by expression (2). It is shown in[4] that the singular part of the free energy F_S is written in the form

$$F_s = \tau_0^{2-\alpha_0} f(\varepsilon/\tau_0^{1/d}), \tag{4}$$

where $f(x)$ is analytic at zero and has a singularity at the point $x = \tilde{A}^{-1/d}$. Using expression (2), we change over in (4) from the variable τ_0 to the variable τ. As a result we obtain

$$F_s = (\tau + \tilde{A}\varepsilon^d)^{2-\alpha_0} f[\varepsilon / (\tau + \tilde{A}\varepsilon^d)^{1/d}]$$
$$= \varepsilon^{d(2-\alpha_0)} (\tilde{A} + \tau / \varepsilon^d)^{2-\alpha_0} [(\tilde{A} + \tau / \varepsilon^d)^{-1/d}]. \quad (5)$$

The function

$$f[(\tilde{A} + \tau / \varepsilon^d)^{-1/d}] = \bar{f}(\tau / \varepsilon^d)$$

has a singularity at the point $\tau/\epsilon^d = \zeta = 0$ and can be represented in the form

$$\bar{f}(\zeta) = \zeta^{2-\alpha}\bar{C}(\zeta), \quad (6)$$

where $\overline{C}(\zeta)$ is a function analytic at the point $\zeta = 0$.

When the perturbation is turned on and d in formula (2) is a non-integer number, the isomorphism may become violated as a result of the change in the exponent α of the perturbed system, or else because of non-analyticity of the function $C(T, \epsilon)$. Let us investigate the analytic properties of $C(T, \epsilon)$ in the simplest case $\alpha = \alpha_0$.

Formula (5) can be rewritten in the form

$$F_s = C(\zeta)\tau^{2-\alpha_0}, \quad (7)$$

where $C(\zeta) = \overline{C}(\zeta)(\tilde{A} + \zeta)^{2-\alpha_0}$ is an analytic function of ζ at the point $\zeta = 0$. We consider the behavior of $C(\zeta)$ as $\zeta \to \infty$. From (7) and (5)

$$C(\zeta) = \tau^{-2+\alpha_0}\varepsilon^{d(2-\alpha_0)} (\tilde{A} + \zeta)^{2-\alpha_0} f[(\tilde{A} + \zeta)^{-1/d}]$$
$$= (1 + \tilde{A} / \zeta)^{2-\alpha_0} f[(\tilde{A} + \zeta)^{-1/d}]. \quad (8)$$

The function $(A + \tilde{A}/\zeta)^{2-\alpha_0}$ is analytic as $\zeta \to \infty$. The argument $(\tilde{A} + \zeta)^{-1/d}$ of the function f goes to 0 as $\zeta \to \infty$, and is analytic with respect to this argument, as stated above. The function $f[A + \zeta)^{-1/d}]$, however, meaning also $C(\zeta)$, will not be analytic in ζ as $\zeta \to \infty$ if $1/d$ is not an integer.

Thus, if $1/d$ is not an integer, the coefficient preceding the singularity of $C(\zeta)$ is a non-analytic function as $\zeta \to \infty$ and cannot be a constant for all $\tau \ll 1$. The characteristic region of variation of C with respect to τ is of the order of ϵ^d.

2. We consider first a system of two interacting Ising spin planes located one above the other. It is shown in[4] that the shift of the critical point due to the interaction ϵ between the planes is proportional to $\epsilon^{4/7}$. Consequently, as shown in the introduction, this interaction violates the isomorphism.

The two-dimensional Ising model with nearest-neighbor interaction J_0 and with interaction along the diagonals J_1 breaks up in the case $\epsilon = J_0/J_1 \ll 1$ into two weakly-interacting sublattices. It is easy to show that in this case the shift of the critical point is proportional to $\epsilon^{4/7}$, and the isomorphism is also violated.

3. We consider a two-dimensional Ising model with interaction along the diagonals in the opposite limiting case $J_1/J_0 \ll 1$. We shall show that in the principal approximation in J_1/J_0 this model is isomorphic to the one considered in[2]. Vaks, Larkin, and Ovchinnikov[2] considered an exactly-solvable planar Ising model with interaction along non-intersecting diagonals (Fig. 1). In the case of weak interaction along the diagonals, the shift of the critical temperature T_c is linear in this interaction and the model turns out to be isomorphic to the Ising model with nearest-neighbor interaction.

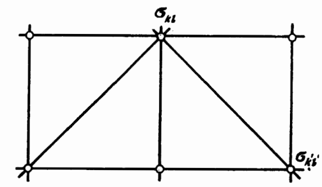

FIG. 1. Ising model with interaction along the diagonals.

The energy E of the system considered in[2] is given by

$$E = E_0 - J_1 \sum_{k,l}{}' \sigma_{kl}\sigma_{k'l'}, \quad (9)$$

where the energy E_0 includes only the nearest-neighbor interaction, the second term of (9) describes the interaction along the diagonals, $\sigma_{kl} = \pm 1$ is the spin variable, and the lattice points are numbered by the indices k and l. The prime at the summation sign denotes that it includes only the lattice points for which $k + l = 2n$.

The partition function of the system under consideration can be expressed in the form

$$Z = \sum_{(\sigma)} \exp\Big(-\frac{E_0}{T} + \sum_{k,l}{}' \bar{\varepsilon}\sigma_{kl}\sigma_{k'l'}\Big)$$
$$= Z_0 \operatorname{ch}^{N/2}\bar{\varepsilon} \sum_{p=0}^{\infty} \frac{\operatorname{th}^p \bar{\varepsilon}}{p!} \sum_{k,l}{}' \langle E'_{k_1 l_1} \ldots E'_{k_p l_p} \rangle, \quad (10)$$

where

$$\bar{\varepsilon} = J_1/T, \quad Z_0 = \sum_{(\sigma)} \exp(-E_0/T), \quad E_{kl}' = \sigma_{kl}\sigma_{k'l'},$$

The sum over k and l takes into account all the permutations of the indices, including those leading to identical expressions.

We express the free energy F in terms of the irreducible correlators Q (see[4,5]):

$$F = F_r + F_0 - T \sum_{p=1}^{\infty} \frac{\operatorname{th}^p \bar{\varepsilon}}{p!} \sum_{k,l}{}' Q(k_1 l_1, \ldots, k_p l_p), \quad (11)$$

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

The characteristic distances in the correlator Q in formula (11) are of the order of the correlation radius of the unperturbed system R_c. The correlators

$$Q(k_1 l_1, \ldots, k_p l_p) = Q(k_1 l_1 + 1, \ldots, k_p l_p) = \ldots = Q(k_1 l_1, \ldots, k_p l_p + 1)$$

are equal accurate to R_c^{-1}.

Consequently, the summation in (11) can be extended over all the points in the following manner:

$$F = F_r + F_0 - T \sum_{p=1} \frac{1}{p!} \frac{\operatorname{th}^p \bar{\varepsilon}}{2^p} \sum_{k,l} Q(k_1 l_1, \ldots, k_p l_p). \quad (12)$$

The summation in (12) is over all the lattice points. This formula coincides with the expression for the free energy of an Ising model with interaction along the diagonals. It is seen from (12) that the shift of T_c in the model of Vaks, Larkin, and Ovchinnikov is half as large at small values of $\bar{\epsilon}$ than in the Ising model with interaction over all the diagonals.

These results, which are obtained with asymptotic accuracy, coincide with the approximate calculations of Fan and Wu[6].

We consider the line of the critical temperatures $T_c(\epsilon)$ in the T, $\epsilon = J_0/J_1$ plane (for a given J_1) (Fig. 2).

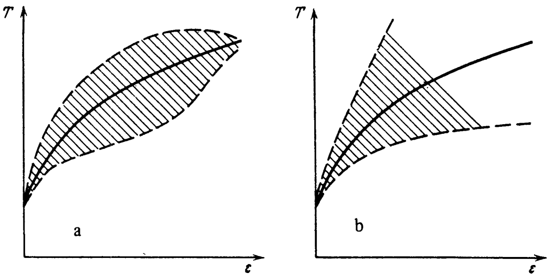

FIG. 2. Possible behavior of the thermodynamic quantities in the Ising model with interaction along the diagonals. The solid line shows the dependence of T_c on ϵ. The thermodynamic quantities behave differently in the shaded and unshaded regions.

In the second section of the present paper we have shown that there is no isomorphism at $\epsilon \ll 1$, and consequently the thermodynamic quantities are described in this region by different formulas inside and outside the cone about the $T_c(\epsilon)$ line, the cone being given by the expression $\tau \sim \epsilon^{4/7}$. As $\epsilon \to \infty$, the cone can behave in one of the following manners.

1) The cone can converge as $\epsilon \to \infty$ (Fig. 2a). In this case the isomorphism obtained in the third section of the present paper and the principal approximation in J_1/J_0 is violated in the next higher orders of approximation.

2) The cone can diverge as $\epsilon \to \infty$ (Fig. 2b). In this case there is actually no cone and isomorphism is conserved.

4. Let us examine the model of a ferromagnet with impurities that are in dynamic equilibrium (the Syozi model[3], Fig. 3). The spin variable σ_i in the M-sublattice, can take on the two values ±1, and the spin variable μ_j in the B-sublattice can take on the three values 0 and ±1.

The energy of such a system is given by

$$E = -J_1 \sum_{i,i'} \sigma_i\sigma_{i'} - J_2 \sum_{i,j} \sigma_i\mu_j - J_3 \sum_{j,j'} \mu_j\mu_{j'} \equiv \bar{E}_0 - J_3 \sum_{j,j'} \mu_j\mu_{j'}. \quad (13)$$

The first term in (13) describes the interaction in the M-sublattice, the second term the interaction between the atom of the main lattice and the impurity, and the third term, which was not taking into account by Syozi [3], describes the direct interaction between the impurity atoms. Without allowance for the last term in (13) in the chemical-potential variable, the Syozi model is isomorphic to the Ising model without impurities[3]. We shall show that this term does not violate the isomorphism at a small impurity concentration $c (c \ll 1)$. The partition function corresponding to the energy (13) can be written in the form

$$Z = \sum_{(\sigma,\mu)} \exp\Big(-\bar{E}/T + B\sum_{j,j'} \mu_j\mu_{j'}\Big), \quad (14)$$

where $\overline{E} = E_0 - \Theta T \Sigma \mu_j^2$, ΘT is the chemical potential of the magnetic ion in the D-sublattice, and $B = J_3/T$.

It is easy to verify the identity

$$\exp(B\mu_j\mu_{j'}) = 1 + x_1\mu_j\mu_{j'} + x_2\mu_j^2\mu_{j'}^2, \qquad x_1 = \operatorname{sh} B, \quad x_2 = \operatorname{ch} B - 1. \quad (15)$$

Taking (15) into account, we rewrite (14) in the form

$$Z = \sum_{(\sigma,\mu)} \exp(-\overline{E}/T) \prod_{j,j'} (1 + x_1\mu_j\mu_{j'} + x_2\mu_j^2\mu_{j'}^2)$$
$$= \sum_{(\sigma,\mu)} \exp\Big(-\frac{\overline{E}}{T}\Big) \sum_{p,q=0}^{\infty} \frac{1}{p!q!} \sum_{j_k, j_k'} x_1^p x_2^q \mu_{j_1}\mu_{j_1'} \ldots \mu_{j_p}\mu_{j_p'}\mu^2_{j_{p+1}}\mu^2_{j'_{p+1}} \ldots$$
$$\ldots \mu^2_{j_{p+q}}\mu^2_{j'_{p+q}}. \quad (16)$$

It can be assumed that all the j_k in the last equation of (16) are different, since the states with coinciding j_k make a small contribution to Z (with respect to the parameter c). We eliminate from (16) the dependence on the variables μ_j:

$$\sum_{\mu_j=0,\pm1} \exp\{G(\sigma_i + \sigma_{i'})\mu_j + \Theta\mu_j^2\} = 1 + 2e^\Theta \operatorname{ch} G(\sigma_i + \sigma_{i'}) = A \exp\{K_1\sigma_i\sigma_{i'}\},$$
$$G = J_2/T, \quad A^2 = (1 + 2e^\Theta \operatorname{ch} 2G)(1 + 2e^\Theta),$$
$$e^{2K_1} = (1 + 2e^\Theta \operatorname{ch} 2G)/(1 + 2e^\Theta),$$
$$\sum_{\mu_j=0,\pm1} \mu_j \exp\{G(\sigma_i + \sigma_{i'})\mu_j + \Theta\mu_j^2\} = 2e^\Theta \operatorname{sh} G(\sigma_i + \sigma_{i'}),$$
$$\sum_{\mu_j=0,\pm1} \mu_j^2 \exp\{G(\sigma_i + \sigma_{i'})\mu_j + \Theta\mu_j^2\} = 2e^\Theta \operatorname{ch} G(\sigma_i + \sigma_{i'}). \quad (17)$$

It is easy to see that

$$\frac{2e^\Theta \operatorname{sh} G(\sigma_i + \sigma_{i'})}{1 + 2e^\Theta \operatorname{ch} G(\sigma_i + \sigma_{i'})} = A_1(\sigma_i + \sigma_{i'}), \quad A_1 = \frac{e^\Theta \operatorname{sh} 2G}{1 + 2e^\Theta \operatorname{ch} 2G},$$
$$\frac{2e^\Theta \operatorname{ch} G(\sigma_i + \sigma_{i'})}{1 + 2e^\Theta \operatorname{ch} G(\sigma_i + \sigma_{i'})} = A_2(1 + x_3\sigma_i\sigma_{i'}),$$
$$A_2 = e^\Theta \frac{\operatorname{ch} 2G + 1 + 4e^\Theta \operatorname{ch} 2G}{(1 + 2e^\Theta)(1 + 2e^\Theta \operatorname{ch} 2G)}, \quad x_3 = \frac{\operatorname{ch} 2G - 1}{\operatorname{ch} 2G + 1 + 4e^\Theta \operatorname{ch} 2G}. \quad (18)$$

We introduce the symbol $E_i = \sigma_i\sigma_{i'}$ for the product of the spins at the nearest neighbors and the symbol $E_i' = \sigma_{i'}\sigma_{i''}$ for products of spins lying on the diagonal (Fig. 3). In this notation, the partition function becomes

$$Z = \sum_{(\sigma)} A \exp\Big(\sum_i KE_i\Big) \sum_{p,q=0}^{\infty} \frac{1}{p!q!} (x_1A_1^2)^p (x_2A_2^2)^q$$
$$\times \prod_{m=1}^{p}\prod_{n=1}^{q}\sum_i (1 + 2E_{i_m} + E'_{i_m})(1 + 2x_3E_{i_n} + x_3^2E'_{i_n})$$
$$= \sum_{(\sigma)} A \exp\Big(\sum_i KE_i\Big) \sum_{p=0}^{\infty} \frac{1}{p!} \sum_i \prod_{m=1}^{p} (v + xE_{i_m} + yE'_{j_m}), \quad (19)$$

where $K = K_1 + J_1/T$, $v = x_1A_1^2 + x_2A_2^2$, $x = 2(x_1A_1^2 + x_3x_2A_2^2)$, $y = x_1A_1^2 + x_3^2x_2A_2^2$. The quantities v, x, and y are of the order of $c^2 = e^{2\Theta}$.

In the last sum of (19), all the indices i_m are different. It is easily seen that the terms with coinciding

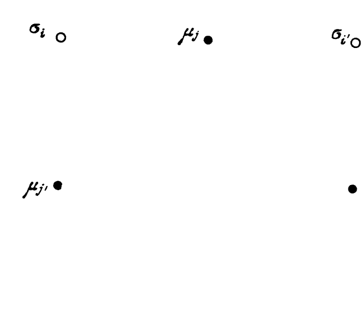

FIG. 3. Ising model with impurities: ○—M-sublattice, ●—D-sublattice.

indices make a small contribution relative to the parameter c^2. Indeed, multiplication of n expressions $v + xE_i + yE'$ with identical indices i yields expressions of the same type, but with coefficients of the order of c^{2n}.

Taking into account the identity

$$\sum_{p=0}^{\infty}\frac{1}{n!}\sum_i\prod_{m=1}^{p} x_{i_m} = \exp\left\{\sum_i x_i\right\},$$

the left side of which contains also terms with identical indices, we obtain from (19)

$$Z=\sum_{(\sigma)} A \exp\left\{\sum_i (KE_i + v + xE_i + yE_i')\right\}$$
$$=\sum_{(\sigma)} \bar{A} \exp\left\{\sum_i (K+x)E_i + \sum_i yE_i'\right\}. \tag{20}$$

As seen from (20), in the principal approximation in c^2 the model under consideration is isomorphic to the Ising model with interaction along the diagonals. As we have seen above, two cases are possible in this Ising model: the isomorphism is either violated in the next-higher approximations, or is conserved in the next higher approximation and an assumption made Fisher[7] and also by Anisimov, Voronel', and Gorodetskiĭ [8] is satisfied, namely that the thermodynamic potential in the variable Θ of a system with impurities is isomorphic to the corresponding thermodynamic potential of the pure substance.

Since the coefficients x and y in (20) are of the order of c^2, the shift of the critical temperature due to the direct interaction is of the order of c^2.

In conclusion the authors thank A. I. Larkin, Yu. N. Ovchinnikov, V. L. Pokrovskiĭ, A. M. Polyakov, and G. V. Ryazanov for valuable discussions.

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Article by V. A. Belinskii, E. M. Lifshitz, and I. M. Khalatnikov, "The Oscillatory Mode of Approach to a Singularity in Homogeneous Cosmological Models with Rotating Axes" (**33**, 1061 (1971)).

In formula (A.7) for P_1^2 the last term in square brackets should be $+2\mu\nu\gamma_{13}\gamma_{23}$.

Article by V. S. Popov, "On the Properties of the Discrete Spectrum for Z Close to 137" (**33**, 665 (1971)).

1. The left side of formula 6 should read

$$xW_{k,\,ig}(x)\ /\ W_{k,\,ig}(x)$$

2. Formula (27′) should read

$$\varepsilon_2(a) = \begin{cases} 2^{-1/2}\left[1+\frac{g}{2}\operatorname{ctg} gL\right] & \text{for} \quad 0 < gL < \pi \\ g\operatorname{ctg} gL & \text{for} \quad \pi < gL < 2\pi \end{cases}$$

Article by Yu. A. Bykovskii, N. N. Degtyarenko, V. F. Elesin, Yu. P. Kozyrev, and S. M. Sil'nov, "Mass Spectrometer Study of Laser Plasma" (**30**, 706 (1971)).

The system of equations (10) should read

$$\begin{aligned} I(z) &\approx \beta_1 \frac{W^{4/9}(\gamma'-1)^{4/9}}{d^{2/3}} \ln\left[\beta_3 z^{1/2}(\gamma'-1)^{1/3}W^{1/3}\right] \\ (\gamma'-1)^{-1} &\approx \frac{3}{2} + \frac{Q(z)}{1+z}\frac{d^{2/3}}{\beta_1(\gamma'-1)^{4/9}W^{4/9}} \end{aligned} \tag{10}$$

Article by Yu. N. Demkov and V. V. Ostrovskii, "n + l Filling Rule in the Periodic System and Focusing Potentials" (**35**, 66 (1972)).

On p. 67, Col. 1, line 2, in the phrase "the larger n at fixed N, the deeper the given level" n should be replaced by l. Correct formulation is implied in the remainder of the text. In the caption of Fig. 3 omit the last words "at the same instant of time." There are also slight errors in Fig. 1 for Z = 41, 43-45, 55-56, and 63-65. In the right hand side of the formula for $f(\nu)$ (Appendix), the denominator should contain the factor $\Gamma(4l + \nu + 1)$ in place of $\Gamma(4l + n_r + 1)$.