объединенный
институт
ядерных
исследований
дубна

E17 - 13016

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2. The Ordered Phase

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Submitted to ТМФ

E17 - 13016

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Сингулярности в критической точке. 2. Упорядоченная фаза

Получены формулы, выражающие восприимчивость в критической области в упорядоченной фазе через параметры вспомогательных гамильтонианов. Анализируется условие критичности. Получены соотношения, связывающие критическое поведение параметра порядка и восприимчивости, из которых при некоторых дополнительных условиях следует известное равенство $\gamma = \beta(\delta - 1)$. Рассмотрение ведется на строгой основе.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1979

E17 - 13016

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Critical-Point Singularities. 2. The Ordered Phase

Some formulas for susceptibility in the ordered phase are obtained, which express its value through parameters of the auxiliary constructions introduced in the Hamiltonian. The critical-point condition is examined. Some relations characterizing the joint behaviour of order parameter and susceptibility are obtained which, under some additional conditions, yield the well-known formula $\gamma = \beta(\delta - 1)$. The method is based on rigorous grounds.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1979

1. Introduction. Here we continue the discussion of the critical behaviour of the many-body systems under the second-order phase transitions started in our previous paper [1]. We shall preserve here general ideas of the approach, and also the notation and numeration of the mathematical statements.

Following [1] we shall use below conventional "magnetic" terminology, calling order parameter "magnetization" and its derivative with respect to the external field "susceptibility". The Hamiltonian of the system to be considered is:

$$H_h = H - hNS \,, \quad h \geqslant 0 \,, \tag{1}$$

where h is the external magnetic field, N is the number of particles (which is proportional to the volume of the system), S is the operator of the magnetisation along the field, H is the Hamiltonian for zero field. Through θ we shall denote the temperature in the energy units ($\theta = kT$). We assume that at the point $\theta = \theta_c$, $h = 0$, where θ_c is the critical temperature, the second-order phase transition takes place (the critical-point condition see below in (5)).

Following [1] we shall denote any system with Hamiltonian Γ and temperature θ as Γ/θ , the quasi-average $\langle S \rangle_{\Gamma/\theta}$ as $S[\Gamma/\theta]$ and the corresponding susceptibility as $\chi[\Gamma/\theta]$ [1)].

1) $\chi[\Gamma/\theta] = \{ dS[\Gamma - hNS/\theta]/dh \}_{h\to 0}$

Let H/θ_c be a critical system, then for the susceptibility in disordered phase the following relation holds true:

$$\chi[H+\rho N S^2/\theta_c] = 1/2\rho \, , \quad \rho > 0. \tag{2}$$

Also, some generalizations of this relation were obtained /1/. In the present paper we derive analogous formulas for the ordered phase, used then to examine the joint behaviour of the order parameter and susceptibility. Under some additional conditions we obtain, in particular, the well-known scaling law $\gamma = \beta(\delta - 1)$. The methods we use are based on rigorous grounds.

Just as in ref./1/ we shall use here as the starting point the "self-consistence" equation for quasi-averages:

$$S[\Gamma/\theta] = S[\Gamma+\rho N S^2 - h N S/\theta]_{h=2\rho S[\Gamma/\theta]}, \tag{3}$$

where parameter $\rho > 0$ is arbitrary. Here the system Γ/θ is arbitrary, whereas the operator S should satisfy the general conditions:

$$\|S\| \le K_1 \, , \quad \|S\Gamma - \Gamma S\| \le K_2 \, , \tag{4}$$

where K_1 and K_2 are constants as $N \to \infty$ and $\|...\|$ means either the norm of an operator (for bounded operators), or the "averaged" norm:

$$\|Y\| = \max_{0 \le h \le h_1} \left(\frac{1}{2} \langle Y\overset{+}{Y} + \overset{+}{Y} Y \rangle_{H-hNS/\theta} \right)^{1/2}, \tag{4a}$$

where $h_1 > 0$ is an arbitrary small fixed positive quantity.

The relation (3) follows from the fundamental "theorem on the free energies" due to N.N.Bogolubov, Jr./2,3/, which in fact expresses some fundamental features of the Gibbs canonical distribution (for more details see Appendix A of ref./1/). We regard below the equation (3) for quasi-averages to be valid. As to the necessary conditions (4), we note that they imply that the order parameter S is of the "quasi-additive" type, and for concrete problems are always valid.

2. Critical-point condition. A generalized critical-point condition has been proposed in ref./1/ For the aim of the present paper, while studying the ordered phase, it is convenient to use a special version of this generalized condition, which we shall refer to as " ζ -condition" (dzeta- condition), originating from the notation in use.

Definition 2 (ζ -critical-point condition). We say that system H/θ_c is at the critical point with respect to the operator S in the sense of " ζ -condition" if [2]

$$M(\zeta) \equiv S[H - \zeta N S^2/\theta_c] = \begin{cases} >0, & \zeta > 0, \\ \to 0, & \zeta \to 0, \end{cases} \tag{5}$$

where for $\zeta > 0$ the function $M(\zeta)$ is assumed to be continuously differentiable and strictly monotonic:

$$dM(\zeta)/d\zeta > 0, \quad \zeta > 0, \quad \zeta \to 0. \tag{5a}$$

These restrictions should be valid in some (may be, small) neighbourhood of the point $\zeta = 0$ for $\zeta > 0$ wherein only the function $M(\zeta)$ should be considered [3].

One can easily see that, as a matter of fact, the critical-point condition itself is (5). The differentiability of $M(\zeta)$ means that the critical point is "solitary", i.e., in the immediate neighbourhood of this point there are no other singular points. As regards the condition $dM(\zeta)/d\zeta > 0$, it should be noted that the condition $dM(\zeta)/d\zeta \ge 0$ is always valid (due to the concavity of the free energy, for more details see footnote 10, in ref./1/) whereas the assumption that $dM/d\zeta = 0$ may occur at the points arbitrary close to $\zeta = 0$ would mean a highly exotic character of the critical point and hence is nonappealing from physical considerations (see also footnote 4 below).

Throughout what follows we assume that for system H/θ_c the ζ -condition is valid.

Let us introduce also in addition to $M(\zeta)$ the function

$$S(h) = S[H - hNS/\theta_c] \, , \quad h > 0, \tag{6}$$

i.e., the function of magnetization for the critical temperature and non-zero field. Note, that in view of (2) the equality holds true:

$$M(\zeta) \equiv S(h = 2\zeta M(\zeta)). \tag{7}$$

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[2] If ref. /1/ we have settled it to choose the positive values for quasi-averages, changing, if necessary, the definition of the initial operator. So, the requirement $M(\zeta) > 0$ here is in fact equivalent to $M(\zeta) \neq 0$.

[3] We shall not mention it below. It will be recalled also that all the conditions necessary when inroducing quasi-averages (in particular, (4)) are supposed to hold true.

Hence it follows that if the τ -condition is valid, then

$$S(h) = \begin{cases} > 0, & h > 0, \\ \to 0, & h \to 0, \end{cases} \tag{8}$$

the function $S(h)$ being continously differentiable and strictly monotonous in some neighbourhood of the point $h = 0$ by $h > 0$:

$$dS(h)/dh > 0, \quad h > 0, \quad h \to 0 \tag{9}$$

(non-strictly monotony being guaranteed ab ovo).

Conditions (5a) and (9) are equivalent. Hereby the violation of (5a) (the assumtion $dM/d\tau = 0$) would mean that as $h \to 0$, one can find such arbitrary small values $h > 0$ that $dS/dh = 0$. Such a behaviour is in contradiction with the common assumption that susceptibility infinitely grows, $dS/dh \to +\infty$, as $h \to 0$[4].

We shall also use below the auxiliary functions /1/:

$$\delta(h) = \frac{S(h)}{h} \Big/ \frac{dS(h)}{dh}, \quad h > 0, \tag{10}$$

$$\delta^*(\tau) = \delta\,(h = 2\tau M(\tau)), \quad \tau > 0. \tag{11}$$

As an important example when the τ -condition holds true one can consider the case of the power asymptotics (with logarithmic corrections) for $S(h)$:

$$S(h) = \left(\frac{h}{D}\right)^{\frac{1}{\delta}} \left| \ln \frac{D'}{h} \right|^{P} (1 + o(h)), \quad o(h) \xrightarrow[h \to 0]{} 0, \tag{12}$$

where $D > 0, D' > 0$; $\delta \geq 1$, P is arbitrary for $\delta > 1$ and $P > 0$ for $\delta = 1$, and where we shall also assume that

$$\begin{cases} h\, do/dh \xrightarrow[h \to 0]{} 0, & \delta > 1; \\ h\,|\ln h|\, do/dh \xrightarrow[h \to 0]{} 0, & \delta = 1, \; P > 0. \end{cases} \tag{12a}$$

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4) As one can see below (see, in particular (21)) the violation of (9) as $h \to 0$ (or (5a) as $\tau \to 0$) means, that every neighbourhood of $h = 0$ contains the points where $dS/dh = 0$ and the points where $dS/dh > R$ for any (arbitrary large) fixed $R > 0$, i.e., in this case $(dS/dh)^{-1}$ has no limit as $h \to 0$ in a common sense (in usual physical cases $(dS/dh)^{-1} \to 0$ as $h \to 0$). It may be interesting to note that the relation (2) holds true even for such an exotic character of the critical point, as the only necessary condition hereby is (5) /1/.

Then for small τ we find from (7) for $\delta > 1$ and $\delta = 1$:

$$M(\tau) = \overline{M}(\tau)(1 + o_\tau), \quad o_\tau \xrightarrow[\tau \to 0]{} 0, \tag{13}$$

$$\overline{M}(\tau) = \left(\frac{\delta}{\delta - 1}\right)^{\frac{P\delta}{\delta-1}} \left(\frac{2\tau}{D}\right)^{\frac{1}{\delta-1}} \left| \ln \frac{D'}{2\tau} \left(\frac{D}{D'}\right)^{\frac{1}{\delta}} \right|^{\frac{P\delta}{\delta-1}}, \quad \delta > 1, \tag{13a}$$

P is arbitrary;

$$\overline{M}(\tau) = \frac{D'}{2\tau} \exp\left\{ -\left(\frac{D}{2\tau}\right)^{\frac{1}{P}} \right\}, \quad \delta = 1, \quad P > 0. \tag{13b}$$

And for $\delta(h)$ (10) we get:

$$\frac{1}{\delta(h)} = \frac{1}{\delta} - \frac{P}{\ln D'/h} + \frac{h\, do/dh}{1 + o(h)}, \tag{14}$$

where δ and P are the critical exponents in (12). Asymptotics for $\delta^*(\tau)$ then follows from (11), (15), and (16).

3. Formulas for susceptibility. Differentiating the identity (7), one finds in notation (11):

$$\frac{dM(\tau)}{d\tau} \Big/ \frac{M(\tau)}{\tau} = \frac{1}{\delta^*(\tau) - 1}. \tag{15}$$

Consider now the function

$$M(\tau + \rho) = S\left[H - (\tau + \rho) N S^2/\theta_c\right], \quad \tau \geq 0, \; \rho > -\tau, \tag{16}$$

for which in virtue of (15)

$$\frac{d}{d\tau} M(\tau + \rho) = M(\tau + \rho) \Big/ (\tau + \rho)(\delta^*(\tau + \rho) - 1). \tag{17}$$

On the other hand, in view of relation (3) the identity holds true:

$$M(\tau + \rho) \equiv S\left[H - \rho N S^2 - 2\tau M(\tau + \rho) N S/\theta_c\right], \quad \tau \geq 0, \; \rho > -\tau. \tag{18}$$

Differentiating this relation with respect to τ and taking into account (17), after some transformations we find the basis formula for susceptibility in the ordered phase:

$$\chi\left[H - \rho N S^2 - h N S/\theta_c\right]_{h = 2\tau M(\tau + \rho)} = \tag{19}$$
$$= \left[2\rho\left(\delta^*(\tau + \rho) - 1\right) + 2\tau\,\delta^*(\tau + \rho)\right]^{-1}, \quad \tau \geq 0, \; \rho > -\tau.$$

The parameters τ and ρ here should satisfy the only restriction $\zeta \geq 0$, $\rho > -\zeta$, being free in other aspects[5]. Let ρ be fixed, then ζ determines the value of the "magnetic field"

$$h = 2\zeta M(\zeta+\rho),\quad \zeta \geq 0,\quad \rho > -\zeta. \qquad (19a)$$

One can also choose the pair ρ and $h \geq 0$ to be independent parameters and obtain the value $\zeta \geq 0$ from equation (19a). As $M(\zeta)$ is monotonic (see (5a)), there exists one-to-one correspondence $h \rightleftarrows \zeta$.

In the case of the power asymptotics for $S(h)$ (12), the formula (19) permits an essential simplification for small ρ and ζ (more precisely, $\zeta+\rho$). Taking into account (12)-(14) we find in this case:

$$\chi\left[H - \rho N S^2 - hNS/\theta_c\right]_{h=2\zeta \bar{M}(\zeta+\rho)} = \qquad (20)$$

$$= \begin{cases} \dfrac{1+O'_{\zeta,\rho}}{2\rho(\delta-1)+2\zeta\delta}, & \delta > 1; \qquad (20a) \\[2ex] \dfrac{D^{1/P}(1+O''_{\zeta,\rho})}{P(2\rho+2\zeta)^{1+1/P}+2\zeta D^{1/P}}, & \delta = 1,\ P>0, \qquad (20b) \end{cases} \qquad \zeta \geq 0,\ \rho > -\zeta,$$

where the function $M(\zeta)$ is defined by (13), and the corrections O' and O'' vanish in the limit $(\zeta+\rho) \longrightarrow 0$.

An important special case of the formulas (19), (20) is that of zero field $h=0$ ($\zeta=0$):

$$\chi\left[H - \rho N S^2/\theta_c\right] = \left[2\rho(\delta^*(\rho)-1)\right]^{-1} = \qquad (21)$$

$$= \left[2\rho(\delta(h)-1)\right]^{-1}\Big|_{h=2\rho M(\rho)},\quad \rho > 0.$$

And for the case of the power-like asymptotics (12), (20) we get:

$$\chi\left[\frac{H-\rho N S^2}{\theta_c}\right] = \frac{1}{\delta-1}\,\frac{1}{2\rho}\left(1+O'_\rho\right),\quad \delta > 1, \qquad (22a)$$

$$\chi\left[\frac{H-\rho N S^2}{\theta_c}\right] = \frac{D^{1/P}}{P}\left(\frac{1}{2\rho}\right)^{1+1/P}\left(1+O''_\rho\right),\ \delta=1,\ P>0, \qquad (22b)$$

$$O'_\rho,\ O''_\rho \xrightarrow[\rho\to 0]{} 0.$$

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[5] However, the value of $\zeta+\rho$ should be such that for $M(\zeta+\rho)$ the ζ-condition (Definition 2) be valid.

Formula (22a) for the susceptibility in the case of the power asymptotics (12) as $\delta > 1$ is quite analogous to (2), the singularity being the same as in (2) $\sim 1/\rho$. Note that in the case $\delta = 1$, $P > 0$ the singularity is stronger than that of (2), see (22b).

Theorem 2. Let for system H/θ_c the ζ-condition with respect to the operator S be valid (see Definition 2). Then for the corresponding susceptibility formulas (19), (21) hold true, and if the stronger version of the critical-point condition (12) is valid, the asymptotical formulas (20), (22) hold true.

4. ζ-Critical-point condition and the behaviour of the functions $S(h)$ and $\delta(h)$.

The definition of the critical state in the form of ζ-condition (5) in terms of $M(\zeta)$, being sufficiently general and technically convenient, possesses some defects because $M(\zeta)$ is not directly ("experimentally") observable quantity. On the other hand, the function $S(h)$ which is connected with $M(\zeta)$ through the equality (7) is of the direct physical sense. Therefore it would be interesting to consider the interrelations of the ζ-condition and the behaviour of the functions $S(h)$ (6) and $\delta(h)$ (10).

Lemma 2. The necessary and sufficient conditions for the ζ-condition to hold true are the following: function $S(h)$ (6) should be continuously differentiable in some neighbourhood of the point $h=0$ for $h>0$ and should satisfy herein the restrictions:

$$S(h) = \begin{cases} >0, & h>0, \\ \to 0, & h \to 0, \end{cases} \qquad (23)$$

$$dS(h)/dh > 0,\quad h > 0, \qquad (24)$$

$$\frac{h}{S(h)} = \left\{\begin{matrix}\text{strictly} \\ \text{monotonuously} \\ \text{increasing} \\ \text{function of } h>0\end{matrix}\right\},\quad \frac{h}{S(h)} \xrightarrow[h\to 0]{} 0. \qquad (25)$$

Hereby the condition (25) (if (23), (24) hold true) is equivalent to the conditions:

$$\frac{dS(h)}{dh} \xrightarrow[h\to 0]{} +\infty, \qquad (26a)$$

$$\delta(h) = \begin{cases} >1, & h>0, \\ \geq 1, & h\to 0, \end{cases} \qquad (26b)$$

where $\delta(h)$ is function (10).

One can easily see that the basic condition here is (25). To prove lemma we start from the equation (7):

$$M(\tau) = S(h = 2\tau M(\tau)). \tag{27}$$

If the τ -condition is valid, then the requirements (23) and (24) are valid, while due to monotony of the function $M(\tau)$ the equation

$$h = 2\tau M(\tau) \tag{27a}$$

defines a single-valued monotonously increasing function $\tau(h)$, $h>0, \tau(h) \to 0$ as $h \to 0$. Putting this function into (27), we find exactly that

$$\tau(h) \equiv h/2S(h). \tag{27b}$$

Hence the requirement (25) is also valid. If, on the other hand, the conditions of the lemma formulated hold true, the relation (27b) defines the unique monotonous function $h(\tau)$, $\tau>0$, $h(\tau)\to 0$ as $\tau \to 0$, and the new function $M(\tau) \equiv S[h(\tau)]$ then satisfies the equation (27) and the requirements of the τ -condition (Definition 2) [6].

Finally, using the definition of the function $\delta(h)$ (10) and rewriting (25) in the form

$$\frac{d}{dh}\left(\frac{h}{S(h)}\right) = \frac{\delta(h)-1}{\delta(h)S(h)} > 0, \quad h > 0, \tag{28a}$$

$$\frac{h}{S(h)} \equiv \frac{1}{\delta(h)(dS(h)/dh)} \xrightarrow[h\to 0]{} +0, \tag{28b}$$

we get sure of the equivalence of the conditions (25) and (26). So lemma 2 is proved.

Let us note that due to (26a) the following identity holds true:

[6] For the sake of completeness, let us also note that equality (27) always has the trivial solution $M(\tau) \equiv 0$ which should be, however, rejected. The quasi-average is just the solution $M(\tau) \neq 0$ (or one of such solutions if there are some nonzero solutions). Indeed, the quasi-average should be calculated from the minimum condition for an auxiliary functional of the free energy $f(C)$, while (27) is the necessary condition of the minimum $\partial f(C)/\partial C = 0$ (for details see /1/). One can easily verify that in view of (25), (26) the miminum is realized just for $M(\tau)\neq 0$. From the physical point of view this means that system "chooses" the thermodynamical phase with spontaneous ordering.

$$1\Big/\frac{dS(h)}{dh}\Big|_{h=h_1} = \int_0^{h_1}\left(-\frac{d^2S}{dh^2}\right)\left(\frac{dS}{dh}\right)^{-2} dh, \quad h \gtrsim 0, \tag{29}$$

where $h_1>0$ can be chosen arbitrary small. One may then conclude that d^2S/dh^2 taken "on the average" should be negative in the neighbourhood of the point $h=0$, for $h \gtrsim 0$, and in any case it cannot be totally positive herein. In other words, the function $S(h)$ should be concave "in average" (in any case not convex) as $h \gtrsim 0$. As regards a special case when d^2S/dh^2 changes its sign as $h \to +0$ whatever small neighbourhood of the point $h=0$ we consider, we then have that $dS/dh \to +\infty$ as $h \to +0$ in the non-monotonous way with the infinitely increasing (as $h \to 0$) frequency of "oscillations". Such an exotic behaviour seems to be unlikely from physical considerations and hardly can occur for usually treated systems (both in theoretical and in experimental studies) which are too simple for such a behaviour. So, limiting oneself only to the physical cases, one can supplement the τ -condition by the requirement of the concavity of $S(h)$ as $h \to 0$ [7]:

$$\frac{d^2S(h)}{dh^2} < 0, \quad h \to +0. \tag{30}$$

5. <u>τ-Condition and classification of critical points.</u> Let us discuss the physical sense of the τ -critical-point condition in more details. Taking into account generally known facts, we can point out two most characteristic aspects of the critical behaviour:

A) The spontaneous long-range order for $\Theta < \Theta_c$ by zero external ordering fields.

B) The divergence of "susceptibilities" (The second derivatives of the free energy) at the critical point.

There is also the following more specific aspect:

C) The power, and sometimes logarithmic, asymptotics are typical for the critical-point behaviour.

As one can easily see, the τ -condition in the form of Lemma 2 represents in part aspect B of the critical behaviour, whereas the τ -condition in its original form of Definition 2 (see (5)) expresses aspect A of the phase transitions. For illustra-

[7] It should be noted that for a wide class of the Ising-type lattices with negative interaction the concavity of magnetization is proved rigorously in ref. /4/.

tion consider system $H-\tau_0 NS^2/\theta_c$ for the concrete case of the Ising-type lattice, when:

$$H=-J\sum_{<i,j>}\sigma_i\sigma_j\,,\quad S=N^{-1}\sum_{1\le i\le N}\sigma_i\,, \tag{31a}$$

$$H-\tau_0 NS^2=-J\sum_{<i,j>}\sigma_i\sigma_j-\frac{\tau_0}{N}\sum_{1\le i,j\le N}\sigma_i\sigma_j\,, \tag{31b}$$

where $J>0$, $\tau_0>0$, $\tau_0\to 0$; $\sigma_i=\pm 1$ and where the sum over $<i,j>$ in (31) is extended only on the nearest neighbours. Let θ_c be the critical temperature for H (31a); it is clear that the decreasing of temperature $\theta_c\to\theta<\theta_c$ is equivalent to the increasing of the interaction $J+\delta J>J$. As one can easily see, the " τ_0-term" in (31b) just models such an intensification of the interaction, with the only difference that this additional interaction (in contrast with that of the initial Hamiltonian) is of the evident long-range type. Nevertheless one can hope that it does not matter much, since in the critical region the effective interaction is of the long-range type in the initial system too [8].

In view of Lemma 2 and the considerations formulated above the aspects A and B of the phase transitions appear to be coupled with each other.

It is interesting also to discuss the relation of τ_0 -condition and aspect C of the critical behaviour. One of the main questions here is about the origins of the characteristic quasi-power asymptotics like in (12), or, in more general form, the question on the existence of the finite limit

$$\delta(h)\xrightarrow[h\to 0]{}\delta\geqslant 1\,. \tag{32}$$

However, as one can easily see the τ_0 -condition itself does not ensure even the boundedness of $\delta(h)$ as $h\to 0$, e.g., the asymptotics

$$S(h)=A_1\left|\ln\frac{A_2}{h}\right|^{-\tau},\quad \tau>0\,,\quad A_1,A_2=const, \tag{33}$$

satisfies τ_0 -condition and even the additional requirement (30), but

8) It should be noted, on the other hand, that for more complex systems (or for more compex order parameters) such a simple correspondence between τ_0-condition and aspect A of the critical behaviour may be destroyed.

$$\delta(h)=\frac{1}{\tau}\left|\ln\frac{A_2}{h}\right|\xrightarrow[h\to 0]{}+\infty\,. \tag{33a}$$

Nevertheless, one can hope, taking into account physical considerations, that in sufficiently simple cases the relation (32) should be valid. Indeed, comparing formulas (2) and (21) we find that only in this case the singularity of susceptibility is the same in ordered and disordered phases [9]. We propose the following interpretation for such a feature: The ordered phase by $\theta=\theta_c(1-\varepsilon)$ differs from the corresponding disordered phase by $\theta=\theta_c(1+\varepsilon)$ (or the system $H-\rho NS^2/\theta_c$ differs from the system $H+\rho NS^2/\theta_c$) only by the existence of the inner "molecular field" (for $\theta<\theta_c$) connected with the spontaneous ordering. The value of this field is in agreement with the value ε (or ρ), so that the effect of the field only renormalizes the "pure temperature" effect, which is the same in two phases [10].

Making use of τ_0 -condition we can classify the critical points (with respect to given order parameter S) by the behaviour of the function $\delta(h)$. The following possibilities are available in the framework of the τ_0 -condition:

I. The function $\delta(h)$ is bounded from above as $h\to 0$:

a) $\delta(h)\xrightarrow[h\to 0]{}\delta>1$,

b)

$$\delta(h)\xrightarrow[h\to 0]{}1,\quad \delta(h)=1+\sigma(h),\quad \sigma(h)=\begin{cases}>0, & h>0,\\ \to 0, & h\to 0.\end{cases}$$

9) Such argument , of course, does not seem too reliable, since in the case $\delta(h)\to 1$, which realizes in practice, the singularity of the susceptibility is different in two phases. As an example, one can consider the two-dimentional Ising model with the order parameter for which the "susceptibility" is really common specific heat. As it is well-known, the specific heat here diverges as $|\ln\varepsilon|$, $h\equiv\varepsilon$, which corresponds to the asymptotics (12) with $\delta=1$, $P>0$. On the other hand, we don't know any concrete examples when $\delta(h)\to+\infty$ as $h\to 0$.

10) In the capacity of the hypothesis we put the assumption that in simple cases such "self-consistency" may be of the nature which is in a sense similar to that of the origins, which leads to the equi-partition of energy on the degrees of freedom.

c) $\delta(h)$ is bounded from below ($1 \le \delta(h)$) and from above, but has no any limit as $h \to 0$ [11].

II. The function $\delta(h)$ is unbounded from above as $h \to 0$:

a) $\delta(h) \xrightarrow[h\to 0]{} +\infty$,

b) $\delta(h)$ has no any limit as $h \to 0$ (i.e. $1/\delta(h)$ does not tend to zero as $h \to 0$).

In the case of the asymptotics Ia and Ib it is convenient to represent the function $S(h)$ in the form:

$$S(h) = h^{1/\delta}\varphi(h), \quad \delta \ge 1, \qquad (34)$$

then

$$\delta(h) = \delta/(1-\omega(h)), \quad \omega(h) \equiv -\delta\cdot\frac{d\varphi}{dh}\Big/\frac{\varphi}{h}, \qquad (34a)$$

where $\varphi(h)$ is a positive function varying strictly slower than by the power law:

$$\omega(h) \xrightarrow[h\to 0]{} 0, \qquad (34b)$$

where in the case $\delta = 1$ it is necessary also to require that

$$\omega(h) > 0, \; h > 0, \qquad \delta = 1. \qquad (34c)$$

As regards the asymptotics Ic , it seems to be not forbidden by the general principles of statistical mechanics, but hardly can occur for real (too simple) systems.

As for the class II (in particular IIa) (see as example (33)), the author doesn't know any concrete examples of the phase transitions with such a behaviour of $\delta(h)$. It is not clear yet, whether this is due to the too simple character of the commonly considered systems and order parameters, or there are more fundamental reasons for such a situation.

6. <u>Special versions of the basic formulas</u>. Choosing the critical system H/θ_c in the basic formulas (19)-(22) in one or another special form, one can get some versions of these formulas handy in applications.

Consider the case, when in virtue of a variation of the Hamiltonian $H \to H+V$ the system leaves the critical point and $H+V/\theta_c$ is noncritical. Let the operator V be of the "ordering" type

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[11] The mathematical example: $\delta(h) = 3 + \sin\frac{1}{h}$.

and can be compensated by introducting into the Hamiltonian of the "disordering" term $+\Delta NS^2$, $\Delta > 0$, by some finite positive value of the parameter $\Delta = \Delta(V) > 0$, so that

$$H+V+\Delta(V)NS^2/\theta_c = \{\text{the } \tau\text{-critical system}\}, \qquad (35a)$$

$$\Delta(V) = \begin{cases} >0, & V \ne 0, \\ \to 0, & V \to 0. \end{cases}$$

In other words (see Definition 2)

$$M_V(\tau) \equiv S[H+V+(\Delta(V)-\tau)NS^2/\theta_c] = \begin{cases} >0, & \tau>0, \\ \to 0, & \tau\to 0, \end{cases} \qquad (35b)$$

where the function $M_V(\tau)$ should be continuously differentiable and rigorously monotonous (see (5a)).

Introduce now for the system (35a), in addition to $M_V(\tau)$, the functions $S_V(h)$, $\delta_V(h)$ and $\delta_V^*(\tau)$, see (6), (10), (11) (where index V labels the system (35a)). Then one can rewrite formulas (19)-(22) and others for the system (35a). In the formulas thus obtained it is especially convenient to choose $\rho = \Delta(V)$. Then, for instance, the basic formula (19) results in

$$\chi[H+V-hNS/\theta_c] = \qquad (36)$$
$$= [2\Delta(V)(\delta_V(h_1)-1) + 2\tau\delta_V(h_1)]^{-1},$$

where

$$h = 2\tau S[H+V-hNS/\theta_c] \ge 0, \qquad (36a)$$

$$h_1 = h + 2\Delta(V)S[H+V-hNS/\theta_c] > 0. \qquad (36b)$$

Here one of the parameters $\tau \ge 0$, $h \ge 0$ is free, deretmining the second one and the parameter h_1 . In particular, we have for $\tau = h = 0$:

$$\chi\left[\frac{H+V}{\theta_c}\right] = \frac{1}{2\Delta(V)}\cdot\frac{1}{\delta[V]-1}, \qquad (37)$$

$$\delta[V] \equiv \delta_V(h = 2\Delta(V)S[H+V/\theta_c]). \qquad (37a)$$

Note also that on the basis of (36) and (37) one can derive the relation:

$$\chi^{-1}\left[\frac{H+V-hNS}{\theta_c}\right] = \frac{\delta_V(h+\ell(V,h))-1}{\delta_V(\ell(V,0))-1}\cdot\chi^{-1}\left[\frac{H+V}{\theta_c}\right] + \qquad (38)$$

$$+\frac{h\cdot\delta_V\left(h+\ell(V,h)\right)}{S[H+V-hNS/\theta_c]}\,,\quad h\geq 0,$$

$$\ell(V,h)\equiv 2\Delta(V)S[H+V-hNS/\theta_c], \qquad (38a)$$

where the parameter $\Delta(V)$ here is the same as in (35).

Let for the functional (37a) the finite limit exists:

$$\lim_{V\to 0}\delta[V]=\delta_0>1\,, \qquad (39)$$

then (37) yields:

$$\chi\left[\frac{H+V}{\theta_c}\right]=\frac{1+O_V}{2\Delta(V)(\delta_0-1)}\,,\quad O_V\xrightarrow[V\to 0]{}0. \qquad (40)$$

As regards the assumption (39), we note that $\delta[V]$ (37a) depends on V in two ways: through the dependence of the function $\delta_V(h)$ on V, and through the dependence h on V. Since for $V=0$ the critical system (35a) coincides with H/θ_c, one can suppose that for a wide class of the initial systems H/θ_c and variations V the functions $\delta_V(h)$ and $\delta(h)$ are close to each other uniformly with respect to h as $V\to 0$ (though for small $h\gtrsim 0$ only)[12]:

$$|\delta_V(h)-\delta(h)|\leq \eta_V\xrightarrow[V\to 0,\,h\gtrsim 0]{}0. \qquad (41)$$

Then the behaviour of $\delta[V]$ as $V\to 0$ is determined by the properties of the function $\delta(h)$ for the initial system. In particular, in the case of the power asymptotics with logarithmic corrections (12) for $\delta>1$ we have in (39) $\delta_0=\delta$ and the relation (40) with $\delta_0=\delta$ is valid, while for $\delta=1$, $p>0$ we get (see (22b)):

$$\chi\left[\frac{H+V}{\theta_c}\right]=\frac{D^{1/p}}{p}\left(\frac{1}{2\Delta(V)}\right)^{1+1/p}(1+O_V),\quad O_V\xrightarrow[V\to 0]{}0. \qquad (42)$$

It should be emphasized that the variation V in the formulas discussed above is not completely arbitrary, but should be of the "weak" type, so that it would be possible to compensate

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[12] In other words, we here assume the function $\delta_V(h)$ to be continuous (with respect to the variational parameter V) when passing from the system H/θ_c to the system $H+V+\Delta(V)NS^2/\theta_c$ (see (35a)). It is intuitively understandable that there are some grounds for such an assumption, if the operators V and ΔNS^2 do not break the symmetry of the initial Hamiltonian H and possess the "ordering" and "disordering" properties which are similar to those of H.

it by the operator ΔNS^2 and to satisfy the condition (35). We shall not discuss here this question in general case, we note only, that for concrete systems it can be often answered just from physical considerations.

Let us for illustration concretize $H+V/\theta_c$ as the initial system by $\theta<\theta_c$, $H/\theta_c(1-\varepsilon)$, $\varepsilon>0$. Let H/θ_c be a simple ferromagnetic system with $\delta(h)\to\delta>1$. One can take, for instance, the Ising-type ferromagnet (see Hamiltonian(31a)). Then it is clear that there exists such finite $\Delta(\varepsilon)>0$ that

$$\frac{H+\Delta(\varepsilon)NS^2}{\theta_c(1-\varepsilon)}=\left\{\begin{array}{c}\text{critical system,}\\ \text{see (5)}\end{array}\right\} \qquad (43)$$

Under the assumption that for system (43) $\delta_\varepsilon(h)\to\delta>1$ as $h,\varepsilon\to 0$, we get for susceptibility:

$$\chi\left[\frac{H}{\theta_c(1-\varepsilon)}\right]=\frac{1}{2\Delta(\varepsilon)}\,\frac{1+O_\varepsilon}{\delta-1}\,,\quad O_\varepsilon\xrightarrow[\varepsilon\to 0]{}0. \qquad (44)$$

<u>Theorem 2A</u>. Let for the system $H+V/\theta_c$, $V\neq 0$ such a finite positive parameter $\Delta(V)>0$ exists that system (35a) satisfies the $\mathcal{C}$-condition. Then for susceptibility formulas (36)-(38) are valid, and under the additional assumption (39) also formula (40) holds true. In a special case of the asymptotics (12) for initial system H/θ_c and under assumption (39) we have for $\delta>1$ formula (40) with $\delta_0=\delta>1$, and for $\delta=1$, $p>0$ formula (42).

7. <u>Relations for critical indices and amplitudes</u>. The above formulas for susceptibility combined with the self-consistency equation (3) make it possible, under some additional conditions, to establish some interrelations in the critical behaviour of magnetization and susceptibility.

Let $H+V/\theta_c$ be the "quasi-critical" system considered in section 6. Making use of (3), we get:

$$S[H+V/\theta_c]=S[H+V+\Delta(V)NS^2-hNS/\theta_c]\Big|_{h=2\Delta(V)S[H+V/\theta_c]} \qquad (45)$$

It is convenient to introduce short notation:

$$S[H+V/\theta_c]\equiv S(V),\quad \chi[H+V/\theta_c]\equiv\chi(V). \qquad (46)$$

Let for the system (35a), occuring on the right-hand side of (45), the assumption (39) $\delta[V]\to\delta_0>1$ be valid. Then for the magnetization on the right-hand side of (45) the power law (34) by $\delta=\delta_0>1$ is valid, and taking into account (45) we get:

$$S(V) = \left[h^{1/\delta_0}\varphi_V(h)\right]_{h=2\Delta(V)S(V)}, V\to 0, \quad (47)$$

where the correction function $\varphi_V(h)$ is continuously differentiable and varies strictly slower than by the power law. Using (40) and keeping only the major term of the asymptotics, as $V\to 0$, we obtain from (47):

$$S(V) = \left[(\delta_0-1)D_0(V)\chi(V)\right]^{-\frac{1}{\delta_0-1}}, V\to 0, \quad (48)$$

$$D_0(V) \equiv \left[\varphi_V(h\equiv S(V)/(\delta_0-1)\chi(V))\right]^{-\delta_0}, \quad (48a)$$

where $D_0(V)$ is a slowly varing function of $S(V)$ and $\chi(V)$.

As a matter of fact, the relation (48) plays the role of the equation of state in the critical region. This formula establishes the connection between the critical behaviour of $S(V)$ and $\chi(V)$ as $V\to 0$, which can be concretized for a concrete behaviour of $S(V)$ and $\chi(V)$.

It is known that for the critical asymptotics the power laws are typical. So let us consider the case, when V is determined by a small parameter $\xi>0, V=V(\xi), V(\xi)\to 0$ as $\xi\to 0$, and suppose that for $S(V)$ and $\chi(V)$ the quasi-power asymptotics hold true:

$$S(V(\xi)) = \xi^{\beta_V} B_V(\xi), \quad \beta_V>0, \quad (49a)$$

$$\chi(V(\xi)) = \xi^{-\gamma_V}\Gamma_V(\xi), \quad \gamma_V>0, \quad (49b)$$

where the "critical indices" β_V and γ_V are constants (subindex V labels the kind of the variation of Hamiltonian), while the amplitude functions $B_V(\xi)$ and $\Gamma_V(\xi)$ vary slower than by the power laws (in the same sense as $\varphi(h)$ in (34)).

Asymptotics as in (49) are typical, for instance, in the case of the temperature variation, when $H+V/\theta_c=H/\theta_c(1-\varepsilon), \varepsilon>0$, the role of ξ hereby plays $\varepsilon>0$[13].

Substituting the asymptotics (49) into (48), we find the relations for critical indices:

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[13] We should note that the notation in (49) is chosen by the analogy with those which are generally accepted in this concrete case.

$$\gamma_V/\beta_V = \delta_0-1, \quad \delta_0\equiv\delta[V]_{V\to 0}>1, \quad (50)$$

and for the amplitude functions:

$$\lim_{\xi\to 0}\left\{(\delta_0-1)D_0(V(\xi))\Gamma_V(\xi)(B_V(\xi))^{\delta_0-1}\right\}=1, \quad (51)$$

where the function $D_0(V)$ is defined in (48a), being connected with the characteristics of the auxiliary system (35a).

Of the major interest is the relation for indices (50). If one accepts the above assumption on the identity $\delta_0=\delta$, where δ is an index for the initial system (see (39), (41)), to hold true, one gets:

$$\gamma_V/\beta_V = \delta-1. \quad (52)$$

This result generalizes the well-known phenomenological "scaling" formula for temperature and field indices (B.Widom, 1964; see, e.g., ref./5/):

$$\gamma' = \beta(\delta-1), \quad (53)$$

where δ is the field index, while the temperature indices γ' and β characterize the behaviour of $\chi(\varepsilon)$ and $S(\varepsilon)$ in the system $H/\theta_c(1-\varepsilon)$, $\varepsilon>0$.

One usually substantiates the relation (53) in the framework of the quasi-phenomenological scaling theory of the critical point, while here we have in fact derived this relation from the "first principles", i.e., from general properties of the Gibbs canonical distribution, on the basis of which all the above results leading to the basic equality (52) have been obtained. Hereby the additional assumptions (on the "weakness" of V, on the indentity $\delta_0=\delta$, etc.) determine in fact the "range of the validity" of the relations like (52), (53)[14].

Note that for all the variations for which in (39) $\delta_0=\delta$ (see also (41)), the quantity γ_V/β_V turns out to be independent of the choice of V. That is because in the critical region $\chi(V)$ is in fact the function of $S(V)$ only.

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[14] One can also choose the inverse order of reasoning and regard numerous experimental confirmations of (53) as an argument in favour of the assumption $\delta_0=\delta$ and other assumptions accepted above.

Theorem 2B. Let H/θ_c be the critical system and $H+V/\theta_c$ be just the system in the ordered phase considered in Theorem 2A, and let condition (39) and relation (40) hold true.

1) Then magnetization and susceptibility for the system $H+V/\theta_c$, $V \to 0$ are linked through the asymptotical relation (48).

2) Let in addition the variation V be determined by a small parameter $\xi > 0$ and let for $\xi \to 0$, $V \equiv V(\xi) \to 0$ the quasi-power asymptotics (49) be valid. Then for critical indices and amplitude functions the relations (50), (51) hold true.

3) For all the variations V which satisfy the assumption $\delta_0 = \delta$, where δ is the field index for initial system H/θ_c, the universal identity for indices (52) is valid.

4) If the temperature variation $V = \varepsilon H$, $\varepsilon > 0, \varepsilon \to 0$ satisfies the conditions announced above in 1-3), then scaling relation (53) holds true.

Acknowledgements:

The author would like to thank Prof. N.N.Bogolubov, Jr. for valuable discussions.

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Received by Publishing Department
on December 21 1979.