объединенный
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ядерных
исследований
дубна

E17 - 12818

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CRITICAL-POINT SINGULARITIES

1. Critical-Point Condition and Susceptibility

1979

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1. Critical-Point Condition and Susceptibility

Submitted to ТМФ

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Сингулярности в критической точке.
1. Условие критичности и восприимчивость.

Обсуждаются равновесные многочастичные системы в критической области. Параметр порядка вводится как квазисреднее, определяемое по методу Н.Н.Боголюбова /мл./. Сформулировано обобщенное условие критичности и обсуждаются специальные случаи этого условия. Получены строгие формулы для восприимчивости в неупорядоченной фазе.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1979

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Critical-Point Singularities
1. Critical-Point Condition and Susceptibility

The equilibrium many-body systems in the critical region are discussed. Order parameter is introduced as the quasi-average defined by the Bogolubov's (Jr.) method. A generalized critical-point condition is formulated and its special cases are examined. Some rigorous formulas for susceptibility in disordered phase are obtained.

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

Preprint of the Joint Institute for Nuclear Research. Dubna 1979

1. Introduction

It is known that under the second-order phase transitions the thermodynamical quantities, characterizing the response of a system on the variation of external parameters, such as specific heat, magnetic susceptibility, compressibility and others, rapidly increase in the critical region and become infinite at the critical point. Such critical singularities appear usually to be of a power or logarithmic type[1]. For instance, the magnetic susceptibility for a temperature near its critical value $\theta \sim \theta_c$ and for zero field $h = 0$ diverges usually as follows:

$$\chi \sim \varepsilon^{-\gamma}, \quad \varepsilon = |\theta - \theta_c| / \theta_c \ll 1, \tag{1}$$

where the value of the critical index γ lies usually between 1 and 2.

Power laws are also typical for the critical behaviour of the "order parameters". So, for spontaneous magnetization by $\theta \to \theta_c$, $h = 0$ the following dependence is typical:

$$M \sim \varepsilon^{\beta}, \quad \varepsilon = (\theta_c - \theta)/\theta_c \ll 1, \tag{2}$$

where for three-dimensional system, as a rule, $\beta \sim 1/3$. Though the order parameters at the critical point become zero, not infinite, their behaviour is in fact singular[2].

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[1] One can regard the logarithmic singularity to be the limiting case of the power one, since $|\ln \varepsilon| = (\varepsilon^{-\alpha} - 1/\alpha)_{\alpha \to 0}$. It should be also noted, that the logarithmic (and even more complex) corrections to pure power laws are possible.

[2] The dependence (2) is non-analytical as $\varepsilon \to 0$. In particular, $dM/d\varepsilon \sim \varepsilon^{\beta - 1} \to \infty$ as $\varepsilon \to 0$, i.e., $dM/d\varepsilon$ demonstrates already the "truly singular" behaviour.

Power laws and related asymptotics seem to be the most profound manifestation of the critical state of a system.

It should be noted that during last decades, due to intensive experimental and theoretical investigations, we have well succeeded in understanding the critical phenomena. In particular, the leading role of fluctuations in the critical-point behaviour has been clarified, the phenomenological concept of scaling has been formulated, some combinatorial methods for approximate calculation of the critical characteristics of simple systems (such as, e.g., Ising-type lattices) have been developed, a set of problems has been analysed by means of the quantum-field-theory methods, and, finally, in the framework of the quasi-phenomenological approach K.Wilson has proposed the ϵ-expansion method for approximate calculation of the critical exponents[3)] (for details see, e.g., refs. /1-4/).

However, a successive microscopic theory of the critical behaviour based on the "first principles" does not exist yet. That is why of a considerable interest for the theory of critical phenomena is the development of approaches and concepts independent of concrete models as well as of phenomenological hypothesis, based on general and rigorously established grounds.

In further papers we shall rigorously discuss some aspects of the critical behaviour concentrating on the analysis of the power and related asymptotics and on the interrelations in the critical behaviour of different quantities. In the present paper we consider the definition of order parameter, and also formulate the generalized critical-point condition and derive some rigorous formulas for susceptibility in disordered phase, which express the susceptibility through parameters of the auxiliary constructions introduced in Hamiltonian (see below (31), (38),(43) and others). In our studies we shall use quite general properties of the Gibbs canonical distribution, estab-

3) We want also to emphasize the important role of the exact solution for the two-dimensional Ising lattice due to L. Onsager (1944). The role of this outstanding theoretical result for progress in studying of critical phenomena in many aspects resembles the role of an important experimental result (though, of cause, this feature of the Onsager's solution does not exhaust its significance).

lished by N.N.Bogolubov, Jr. when studying the superconducting model systems (see refs. /6-8/ and Appendix A).

2. The Phase Transition

We shall consider the second-order phase transitions with the singular behaviour of the one-component real order parameter. For the sake of simplicity let us speak on the ferromagnetic phase transition, calling the order parameter "magnetization" and its derivative with respect to the external field "susceptibility". Naturally, all the formal results derived below permit any other physical interpretation.

Let H be the Hamiltonian of such a "ferromagnetic" system at zero field $h=0$. For $h>0$ the Hamiltonian will be:

$$H_h = H - hNS\ , \quad S = S^+, \quad h > 0\ , \tag{3}$$

where S is the operator of magnetization along the field (per particle), N is the number of particles (magnetic moments) in the system, proportional to its volume V . By θ we shall denote the temperature in energy units, $\theta = kT$. Let $M(\theta,h)$ and $\chi(\theta,h)$ be "magnetization" and "susceptibility" for our system:

$$M(\theta,h) = \langle S \rangle_{H_h,\theta} = -df(\theta,h)/dh, \tag{4}$$

$$\chi(\theta,h) = dM(\theta,h) = -d^2f(\theta,h)/dh^2, \tag{5}$$

where $\langle\dots\rangle_{H_h,\theta}$ is the equilibrium Gibbs average and $f(\theta,h)$ is the free energy of a system[4].

At the critical point $\theta=\theta_c$, $h=0$ the second-order phase transition occurs: The spontaneous magnetization $M(\theta,h=0)$ goes continuously to zero as $\theta\to\theta_c$ by $\theta<\theta_c$ and remains zero for all $\theta\geqslant\theta_c$, while the susceptibility becomes $+\infty$ at the critical point (irrespective of the "trajectory" on the $\theta-h$ plane, along which the system approaches the critical point).

As an example of such a system, one may consider the Ising-type ferromagnetic model with the Hamiltonian:

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4) The definition: for an arbitrary system with Hamiltonian Γ and temperature θ

$$f[\Gamma,\theta] = -\frac{\theta}{N}\ln \mathrm{Tr}\, e^{-\Gamma/\theta}, \quad \langle\dots\rangle_{\Gamma,\theta} = \mathrm{Tr}(\dots e^{-\Gamma/\theta})/\mathrm{Tr}\, e^{-\Gamma/\theta},$$

where "Tr" is the trace over the whole space of states of a system, N is the number of particles proportional to the volume of a system V.

$$H = -\sum_{1\le i,j\le N} J_{ij}\sigma_i\sigma_j - h\sum_{1\le i\le N}\sigma_i\ , \quad S = N^{-1}\sum_{1\le i\le N}\sigma_i \tag{6}$$

where $\sigma_i = \pm 1$, $J_{ij} > 0$ for the nearest neighbours (or some "strata" of the nearest neighbours) and $J_{ij} = 0$ for distant neighbours. For $d=2$ and $d=3$ (d is dimention) in such systems the phase transition of the type described above takes place.

3. Order Parameter and Quasi-Averages

We want to note, following the classical paper by N.N.Bogolubov/5/, that the order parameter should be always defined with taking into account symmetry-breaking effects. For instance, the spontaneous magnetization for model (6) should be defined as the quasi-average $\prec S \succ$, rather than the usual Gibbs average $\langle S\rangle$ by $h=0$ in the limit $N\to\infty$. Accepting the canonical definition of the quasi-averages/5/, we have:

$$\prec S \succ_{H,\theta} = \lim_{h\to 0}\lim_{N\to\infty} \langle S\rangle_{H_h,\theta}\ , \tag{7}$$

where $N\to\infty$ means thermodynamical limit[5]; the sequence of limits is here essential. The physical meaning of the definition (7) is obvious: the spontaneous magnetization should be calculated by the infinitesimal external magnetic field being switched on, the field fixes the direction of spontaneous magnetization. However, in spite of the clear physical meaning, such a definition may appear to be not effective enough in the general case, when the Hamiltonian and the state of a system are not defined in detail.

New effective methods in the theory of quasi-averages have been developed by N.N.Bogolubov, Jr. when studying superconducting models/7,8/. These methods are based on the fundamental theorem on the functional of the free energy/6/ (the mathematical formulation of the Theorem see in Appendix A). Here we shall discuss it shortly from the point of view appropriate for our further needs.

Let Γ be an arbitrary Hamiltonian. Introduce also the Hamiltonian:

$$\Gamma_\rho(C) = \Gamma + \rho N (S - C)^2, \quad \rho > 0, \tag{8}$$

where C is a variational parameter, $S = S^+$ is some operator construction, which should satisfy the only conditions:

$$\| S \| \le K_1\ , \quad \| S\Gamma - \Gamma S \| \le K_2\ , \tag{9}$$

where $\|\dots\|$ means the norm of the operator, K_1 and K_2 are cons-

5) Thermodynamical limit: $N\to\infty$, $V\to\infty$, $N/V = $ constant, where N is the number of particles, V is the volume of a system.

tants[6]. Let us calculate the free energy for the system with the Hamiltonian (8) in the limit $N \to \infty$ (for some fixed temperature θ, which we shall not indicate) and then minimize it with respect to C. Denote the minimizing value of C as $\bar{C}$,

$$f_\infty[\Gamma_\rho(\bar{C})] = \operatorname{abs}\min_C \left(\lim_{N\to\infty} f_N[\Gamma_\rho(C)] \right). \quad (10)$$

Then the Bogolubov, Jr.'s theorem yields that in the thermodynamical limit ($N \to \infty$) the free energy for the basic system (Γ, θ) coincides with that of (10) for every $\rho > 0$ and every fixed $\theta \geqslant 0$:

$$\left| f_N[\Gamma] - f_\infty[\Gamma_\rho(\bar{C})] \right| \xrightarrow[N \to \infty]{} 0. \quad (11)$$

Furthermore, parameter $\bar{C}$ in (10) does not depend on $\rho > 0$, and, consequently, one can regard $\bar{C}$ to be the quasi-average $\langle S \rangle_{\Gamma,\theta}$,

$$\bar{C} = \langle S \rangle_\Gamma. \quad (12)$$

If equation (10) provides more than one value for $\bar{C}$, one should fix one of them to be the quasi-average (here we have the same situation, as in the choice of the direction of spontaneous magnetization).

Making use of the minimum condition (10), one can easily obtain that the quasi-average (12) satisfies the "self-consistence equation" [7]

$$\bar{C} = \langle S \rangle_{\Gamma_\rho(\bar{C})}, \quad \bar{C} \equiv \langle S \rangle_\Gamma, \quad \rho > 0. \quad (13)$$

which is just the result we only need below (see also Appendix A).

It should be emphasized that the results described above are independent of any details of the concrete structure of the operators Γ and S. So, the Bogolubov, Jr.'s Theorem demonstrates some universal "mathematical" properties of the Gibbs canonical ensemble[8]. One can apply these general properties when consider-

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[6] One can, if necessary, weaken the conditions (9), requaring the operators in (9) to be bounded not in norm, but only "in average", for details see Appendix A, (A11).

[7] Let us note, in order to illustrate the physical meaning of equation (13), that of the same nature are the molecular-field equations in the theory of magnetizm, the gap equation in the theory of superconductivity, etc.

[8] Here we have one more manifestation of a well-known deep physical principle "of minimum of energy".

ing different problems in the equilibrium many-body theory[9]. As regards the present paper, we shall use equality (13) as a starting point to prove some special formulas for susceptibility in systems with the second-order phase transitions. It is of particular importance for our aim that hereby the problem of the effective definition of the quasi-averages appears to be solved automatically.

Taking the problem in general, we want to note that because of the close connection between phase-transitions and symmetry-breaking effects, essential restrictions exist for the methods of general analysis of the critical behaviour, when the system considered is not concretized in all details. Namely, for all such methods the order parameter should be considered in the sense of quasi-averages. From our point of view, the most convenient (if not the only possible) to this end is the definition of the quasi-averages in accordance with the described procedure (see (12)). That is why the relations (12),(13), taken as a starting point for our studies, are inevitable in many aspects.

4. New Notation

Let us denote by Γ/θ an arbitrary system with Hamiltonian Γ and temperature θ , and use this notation as a functional argument. In particular, we shall denote the quasi-average $\langle S \rangle_{\Gamma,\theta}$ by $S[\Gamma/\theta]$ and the corresponding susceptibility by $\chi[\Gamma/\theta]$.

In this notation one can represent the equality (13) as follows:

$$S[\Gamma/\theta] \equiv S[\Gamma + \rho N S^2 - h N S]_{h = 2\rho S[\Gamma/\theta]} \tag{14}$$

Throughout what follows when making use of quasi-averages and equality (14), we consider (without special remarks) all the necessary conditions, in particular conditions (9) or their generalizations, to be satisfied. We shall also consider (for the sake of convenience) the quasi-averages $S[\Gamma/\theta]$ to be usually non-negative quantities. One can always get this end, changing, if necessary, the sign of the initial operator $S \to -S$. It should be also noted, that if $S[\Gamma/\theta]$ is really the spontaneous magnetization, there is the symmetry between positive and negative choice

9) One can consider, as an example, the methods of the asymptotically exact solution for some classes of model Hamiltonians /6-9/. Just when studying that range of problems the basic Theorem (11) has been proved /6/.

of the quasiaverage $S[\Gamma/\theta]$; so we shall always choose the positive value for the spontaneous magnetization.

5. The Critical-Point Condition

Here we shall consider the definition of the critical point for the case of the second-order phase transitions. Let us return to the "magnetic" therminology of section 2 and consider the system with Hamiltonian (3). Let H be the zero-field Hamiltonian; S, the order parameter operator; θ_c, the critical temperature. If H/θ_c is the critical system, we have:

$$S[H/\theta_c] = 0, \tag{15a}$$

$$\chi[H/\theta_c] = +\infty. \tag{15b}$$

These equalities should be valid whatever the definition for the critical point is accepted.

As a formal generalized definition of the critical point (critical-point condition) we propose the following:

Definition 1. We say that the system H/θ_c is at the critical point with respect to the operator S, if there exists such a variation of the Hamiltonian $H \to H+\delta H$, that the following conditions are satisfied:

$$S[H+\delta H/\theta_c] = \begin{cases} \neq 0, & \delta H \neq 0, \\ \to 0, & \delta H \to 0, \end{cases} \tag{16a}$$

$$S[H+\delta H+\rho N S^2/\theta_c] \Big/ S[H+\delta H/\theta_c] \xrightarrow[\delta H \to 0,\ \rho>0]{} 0, \tag{16b}$$

where (16b) has to be valid for every (arbitrary small) fixed $\rho > 0$.

The quasi-averages are here supposed to be defined by (12), the equality (14) being valid (the operators $H, \delta H, S$ should satisfy all necessary conditions, see (9)). It should be noted that from the physical point of view the basic conditions (9) imply only the "quasi-additive" character of the order parameter and always hold true for concrete systems (see also footnote 6).

Two notes to Def. 1.

1) If the condition (16b) is valid for some fixed $\rho=\rho_0>0$, it is valid also for all $\rho>\rho_0$. That is due to the fact that the modulus of the numerator of (16b) never increases as ρ grows[10].

10) Irrespective of system Γ/θ and of operator A the inequality $d^2 f[\Gamma+xNA/\theta]/dx^2 \leq 0$ or $dA[\Gamma+xNA/\theta]/dx \leq 0$ holds true (the concavity of the free energy). In particular, always $dS^2[\Gamma+\rho N S^2/\theta]/d\rho \leq 0$. Taking also into account that $S^2[\dots] = |S[\dots]|^2$ (Appendix A (A10)), we find that the modulus of the numerator in (16b) decreases monotonously with growing ρ.

2) Making use of the concept of variational derivatives, one can rewrite (16b) (if (16a) is valid) into the form [11]:

$$\frac{\delta S[H+\rho NS^2/\theta_c]/\delta H}{\delta S[H/\theta_c]/\delta H} = 0, \quad \rho > 0. \tag{17}$$

Note that the critical-point conditions (16) ensure the properties (15) to hold true. In particular, (15b) is valid owing to (31) (see below).

It should be also noted that the critical condition (16) is broader than the generally accepted quasi-phenomenological concept of the second-order phase transition critical point. In particular, the condition (16)may hold true also in some special singular points, which are not usually regarded to be the phase transition points. The points where a system loses its thermal stability seem to be the possible candidates on this role.

Consider now some concrete physical examples for the choice of the variation δH in the critical conditions (16) [12].

A. Choosing in (16) $H+\delta H/\theta_c$ in the form $H-hNS/\theta_c$, one can rewrite the critical-point conditions as

$$S[H-hNS/\theta_c] = \begin{cases} >0, & h>0, \\ \to 0, & h\to 0, \end{cases} \tag{18a}$$

$$\chi[H+\rho NS^2/\theta_c] = \begin{cases} \neq\infty, & \rho>0, \\ \to\infty, & \rho\to 0. \end{cases} \tag{18b}$$

To confirm (18) let us note that due to (14) the following rule is always valid:

$$S[\Gamma/\theta] \to S[\Gamma+\rho NS^2/\theta] = 0, \quad \rho > 0, \tag{19}$$

where the arrow means that the left-hand equality with necessity leads to the right-hand one. So, if the conditions (18) hold true, then $S[H/\theta_c] = S[H+\rho NS^2/\theta_c] = 0$, and making use of the definition (5) we get:

$$\lim_{h\to 0} \frac{S[H-hNS+\rho NS^2/\theta_c]}{S[H-hNS/\theta_c]} = \frac{\chi[H+\rho NS^2/\theta_c]}{\chi[H/\theta_c]} = 0.$$

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11) It should be noted that such a representation is rather formal, since the ratio (17) may appear to be of the type ∞/∞ or $0/0$. However, we shall not discuss here this question in more detail, since below we deal directly with (16). Note, on the other hand, that the condition (17) is of a certain physical obviousness: here one can easely see, that the critical system is anomalous sensitive with respect to the variation of the Hamiltonian δH, while the term ρNS^2 removes this anomalous sensitiveness.

12) On the other hand, the case when δH has no any appropriate physical meaning is also possible.

So both conditions (16) are satisfied.

B. One can also choose $H+\delta H/\theta_c$ to be the initial system by $\theta < \theta_c$, i.e., $\theta = \theta_c(1-\varepsilon)$, $\varepsilon > 0$. Then the critical conditions (16) get the form:

$$S[H/\theta_c(1-\varepsilon)] = \begin{cases} >0, & \varepsilon > 0 \\ \to 0, & \varepsilon \to 0 \end{cases}, \qquad (20a)$$

$$S[H+\rho NS^2/\theta_c(1-\varepsilon)]/S[H/\theta_c(1-\varepsilon)] \xrightarrow[\varepsilon\to 0,\ \rho>0]{} 0. \qquad (20b)$$

In particular, the condition (20b) is satisfied, if the "demagnetization" term ρNS^2 in the Hamiltonian makes the critical temperature lower by a finite quantity, $\theta_c \to \theta_c(\rho) < \theta_c$. Then for sufficiently small $\varepsilon > 0$, such that $\theta_c(\rho) < \theta_c(1-\varepsilon) < \theta_c$, the numerator in (20b) becomes zero and (20b) is valid.

C. If one chooses $H+\delta H/\theta_c$ in the form $H - \tau NS^2/\theta_c$, $\tau > 0$, the critical-point condition (16a) takes the form:

$$M(\tau) \equiv S[H-\tau NS^2/\theta_c] = \begin{cases} >0, & \tau > 0, \\ \to 0, & \tau \to 0. \end{cases} \qquad (21)$$

Here the "ferromagnetic" term $-\tau NS^2$ is introduced in the Hamiltonian, which favours the ordering. The condition (21) then means that such a term makes the critical temperature higher by a finite quantity. The condition corresponding to (16b) is the following:

$$\lim_{\tau\to 0} \frac{S[H+(\rho-\tau)NS^2/\theta_c]}{S[H-\tau NS^2/\theta_c]} = 0, \quad \rho > 0.$$

This condition holds true automatically, since for all $0 \le \tau \le \rho$ the denominator here is identically zero (due to (19)).

D. One can also verify that the critical-point conditions (16) are valid if the magnetization for nonzero magnetic field satisfies the standard power law (with possible logarithmic correction):

$$S[H-hNS/\theta_c] = \left(\frac{h}{D}\right)^{\frac{1}{\delta}} \left|\ln\frac{D'}{h}\right|^{p} (1+o(h)), \quad h \geqslant 0, \quad o(h) \xrightarrow[h\to 0]{} 0, \qquad (22)$$

where δ, p, D, D' are real parameters, $D > 0$, $D' > 0$, $\delta \geqslant 1$; the parameter p is arbitrary ($-\infty < p < +\infty$) for $\delta > 1$, and $p > 0$ for $\delta = 1$.

In virtue of (14) the quasi-average $M(\tau)$ (21) satisfies the relation:

$$M(\tau) = \left[\left(\frac{h}{D}\right)^{\frac{1}{\delta}} \left|\ln\frac{D'}{h}\right|^{p} (1+o(h))\right]_{h=2\tau M(\tau)} \qquad (23)$$

whence we find for $\delta > 1$ and $\delta = 1$

$$M(\tau) = \bar{M}(\tau)(1+O_\tau), \quad O_\tau \xrightarrow[\tau\to 0]{} 0, \qquad (24)$$

where

$$\begin{cases} \overline{M}(\tau) = \left(\frac{\delta}{\delta-1}\right)^{\frac{p\delta}{\delta-1}} \left(\frac{2\tau}{D}\right)^{\frac{1}{\delta-1}} \left| \ln \frac{D^*}{2\tau} \right|^{\frac{p\delta}{\delta-1}}, \\ \delta > 1, \; p \text{ is arbitrary}, D^* = D^{1/\delta} D'^{\frac{\delta-1}{\delta}}; \end{cases} \tag{24a}$$

$$\overline{M}(\tau) = \frac{D'}{2\tau} \exp\left\{-\left(\frac{D}{2\tau}\right)^{1/p}\right\}, \; \delta = 1, \; p > 0. \tag{24b}$$

So, the condition (21) is satisfied and hence the generalized critical condition (16) holds true.

6. The Basic Formula for Susceptibility

Let H/θ_c be the critical system in the sense of Definition 1 and let $H+\delta H/\theta_c$ be the auxiliary system herein. Introduce also the auxiliary Hamiltonian

$$H_\delta(\rho, h) = H + \delta H + \rho N S^2 - h N S, \; \rho > 0, \; h > 0, \tag{25}$$

and denote through $M_\delta(\rho, h)$ and $\chi_\delta(\rho, h)$ magnetization and susceptibility for the system $H_\delta(\rho,h)/\theta_c$. Averaging the equality

$$\chi_\delta(\rho, h) = d M_\delta(\rho, h)/dh \tag{26}$$

over h from 0 till $h_1 \neq 0$, we get

$$\chi_\delta(\rho, \bar{h}) = \frac{1}{h_1}\left[M_\delta(\rho, h_1) - M_\delta(\rho, 0)\right], \; 0 \le |\bar{h}| \le |h_1|. \tag{27}$$

Choosing here

$$h_1 = 2\rho S[H + \delta H/\theta_c] \neq 0, \; \delta H \neq 0, \tag{28}$$

and taking into account that owing to the universal "self-consistence" equality (14)

$$M_\delta(\rho, h_1 = 2\rho S[H+\delta H/\theta_c]) \equiv S[H + \delta H/\theta_c] \tag{29}$$

one obtains from (27):

$$\chi\left[H + \delta H + \rho N S^2 - \bar{h}_{\delta,\rho} N S/\theta_c\right] = \frac{1}{2\rho}\left(1 - \frac{S[H+\delta H + \rho N S^2/\theta_c]}{S[H+\delta H/\theta_c]}\right), \tag{30}$$

$$0 \le |\bar{h}_{\delta,\rho}| \le 2\rho\,|S[H+\delta H/\theta_c]|.$$

Passing here to the limit $\delta H \to 0$ and taking into account the critical conditions (16), we finally get our basic formula for susceptibility:

$$\chi\left[\frac{H + \rho N S^2}{\theta_c}\right] = \frac{1}{2\rho}, \; \rho > 0. \tag{31}$$

Here the parameter ρ is an arbitrary (not necessary small) positive quantity. Note also, that for $\rho \to 0$ we have $\chi[H/\theta_c] = +\infty$, just in agreement with (15b).

So, we have proved the following statement:

<u>THEOREM 1</u>. Let system H/θ_c be at the critical point with respect to the operator S (in the sense of Definition 1). It is sufficient to assume, in particular, that any of special critical

conditions (18), (20), (21) or (22) is valid. Then for the susceptibility corresponding to the operator S formula (31) holds true.

7. Generalized Formulas for Susceptibility

In a special case of the power-like asymptotics (22) one can easily generalize the basic formula (31) to the case of non-zero weak magnetic field.

We consider first even more general case when the critical condition is taken in the form (21) for the quasiaverage $M(\tau)$. As regards $S(h)$ we shall assume only that

$$S(h) \equiv S[H - hNS/\theta_c] = \begin{cases} >0, & h>0, \\ \to 0, & h \to 0. \end{cases} \qquad (32)$$

Note that due to the self-consistency equation (14) $M(\tau)$ satisfies the equality:

$$M(\tau) \equiv S[H + \rho NS^2 - 2(\rho+\tau)M(\tau)NS/\theta_c], \quad \tau \geq 0, \; \rho \geq 0, \qquad (33)$$

in particular, for $\rho = 0$ we have:

$$M(\tau) \equiv S(h = 2\tau M(\tau)), \quad \tau \geq 0. \qquad (34)$$

So, (32) is a consequence of the critical condition (21) (the inverse conclusion is wrong).

We shall suppose below the functions $M(\tau)$ and $S(h)$ to be continuously differentiable for all $\tau > 0$, $h > 0$ in some neighbourhood of the singular point $\tau = 0$, $h = 0$ (wherein only these functions to be considered).

Let us also introduce new functions:

$$\delta(h) = \frac{S(h)}{h} \Big/ \frac{dS(h)}{dh}, \quad h > 0, \qquad (35)$$

$$\delta^*(\tau) = \delta(h = 2\tau M(\tau)), \quad \tau > 0. \qquad (36)$$

Differentiating the identity (34) we get in this notation:

$$\frac{dM(\tau)}{d\tau} \Big/ \frac{M(\tau)}{\tau} = 1/(\delta^*(\tau) - 1), \quad \tau > 0. \qquad (37)$$

On the other hand, differentiating (33) and making use of (37), after some transformations we obtain the formula generalizing (31):

$$\chi[H + \rho NS^2 - hNS/\theta_c]_{h = 2(\rho+\tau)M(\tau)} = \qquad (38)$$
$$= 1/(2\rho + 2\tau\delta^*(\tau)), \quad \tau \geq 0, \; \rho > 0.$$

Note that parameters $\tau \geq 0$ and $\rho > 0$ hereby are arbitrary (not necessary small). Instead of ρ and τ one can also choose ρ and h, $\rho > 0$, $h \geq 0$, to be independent parameters. Then one should calculate τ from the equation:

$$h = 2(\rho+\tau)M(\tau),\ \rho>0,\ h\geq 0. \qquad (38a)$$

Since $M(\tau)$ is a monotonously increasing function [13], the equation (38a) provides the one-to-one correspondence $h \rightleftarrows \tau$ ($h\geq 0$, $\tau \geq 0$).

Formula (38) permits a simplification in the case when the power-like asymptotics (22) holds true. Then for $M(\tau)$ we have the relations (24), and for $\delta(h)$ (35) we get:

$$\frac{1}{\delta(h)} = \frac{1}{\delta} - \rho \Big/ \ln\frac{D'}{h} + \frac{h\, dO/dh}{1+O(h)}, \qquad (39)$$

where δ is the critical index in (22). Asymptotics for $\delta^*(\tau)$ then follows from (36) and (39). Assuming the correction $O(h)$ in (22) to be a sufficiently "smooth" function, such that in (39)

$$|h\, dO/dh| \xrightarrow[h\to 0]{} 0, \qquad (39a)$$

we finally get $\delta(h)\to\delta$, $\delta^*(\tau)\to\delta$ as $h\to 0$, $\tau\to 0$. Hence, formula (38) yields:

$$\chi\left[H+\rho NS^2 - hNS/\theta_c\right]_{h=2(\rho+\tau)M(\tau)} = \qquad (40)$$

$$= 1\Big/\left(2\rho+2\tau\cdot\delta\cdot(1+O_\tau)\right),\ \tau\geq 0,\ \rho>0,\ O_\tau \xrightarrow[\tau\to 0]{} 0,$$

where $\delta \geq 1$ is the critical index in (22), $\bar{M}(\tau)$ is represented by (24), $\bar{M}(\tau)\to 0$ as $\tau\to 0$.

So, the following statement holds true:

THEOREM 1A. Let system H/θ_c be at the critical point with respect to the operator S in the sense of the special critical condition (21), and let the functions $M(\tau)$ (21) and $S(h)$ (32) be continuously differentiable in some neighbourhood of the point $\tau=0$, $h=0$ for $\tau>0$, $h>0$. Then in this neighbourhood for the susceptibility corresponding to the operator S formula (38) is valid. In the case of the stronger version of the critical condition, when the conditions (22) and (39a) are valid, the asymptotical formula (40) holds true.

8. Some Other Versions of the Basic Formulas

The system H/θ_c in the formulas derived above should satisfy only the critical condition, being free in other aspects. Hence, choosing the critical system H/θ_c in one or another concrete form, one can obtain different modifications of the basic formulas.

Consider the situation when through the variation of the Hamiltonian $H\to H+W$ the critical system H/θ_c passess to non-critical

13) In virtue of the convexity of the free energy $dM/d\tau\geq 0$, see footnote 10.

one $H+W/\theta_c$. Let the variation be of the "disordering"type and can be compensated by the "ordering" term $-\Delta NS^2$ by a finite positive value of the parameter $\Delta = \Delta(W) > 0$, so that the resulting system becomes the critical one again:

$$\frac{H+W-\Delta(W)NS^2}{\theta_c} = \left\{ \begin{array}{l} \text{the critical system} \\ \text{in the sense of Def.1} \end{array} \right\} \quad (41)$$

$$\Delta(W) = \begin{cases} >0, & W \neq 0, \\ \to 0, & W \to 0. \end{cases} \quad (41a)$$

Note that the condition (41) holds true if (see (21)):

$$S\left[H+W-(\Delta(W)+\tau_0)NS^2/\theta_c\right] = \begin{cases} >0, & \tau_0>0 \\ \to 0, & \tau_0 \to 0. \end{cases} \quad (42)$$

One can easily verify that the system $H+W/\theta_c$ is really in the disordered phase: starting with $S[H+W-\Delta(W)NS^2/\theta_c]=0$ and taking into account (19), one obtains

$$S[H+W/\theta_c] = 0, \quad W \neq 0.$$

One can rewrite the basic formulas (31) and (if the corresponding conditions are valid) (38),(40) for the case (41),(42), the term $-\Delta(W)NS^2$ being then compensating (completely or in part) by the term ρNS^2. In particular, on the basis of (31) and (41) we get:

$$\chi\left[\frac{H+W}{\theta_c}\right] = \frac{1}{2\Delta(W)}, \quad (43)$$

where the parameter $\Delta(W)$ is definite in (41). Note also that in view of (31) and (41) the following relation holds true:

$$\chi[H+W/\theta_c] = \chi\left[H + \tfrac{1}{2}\chi^{-1}[H+W/\theta_c]\cdot NS^2/\theta_c\right]. \quad (43a)$$

Let (42) be valid, then making use of (33)-(36),(38),(43) one can easily derive the relation:

$$\chi^{-1}(W,h) = \chi^{-1}(W,0) + \chi_W^{-1}(0, h_1 = h - \chi^{-1}(W,0)S(W,h)), \quad (44)$$

where

$$\chi(W,h) = \chi[H+W-hNS/\theta_c],$$
$$S(W,h) = S[H+W-hNS/\theta_c],$$
$$\chi_W(0,h_1) = \chi[H_W - h_1 NS/\theta_c],$$
$$H_W \equiv H+W-\Delta(W)NS^2, \quad H_W/\theta_c = \text{the critical system}(41).$$

Note that for any fixed $W \neq 0$ and $h \to 0$ in (44) $h_1 \sim h^2$:

$$h_1 = h^2\left\{-\frac{d\chi(W,h)}{dh}\Big/2\chi(W,h)\right\}_{h=0} + O_W(h^3), \quad (44a)$$

$$O_W(h^3) \sim h^3 \quad \text{as } h \to 0, \ W \neq 0.$$

The analogous considerations are valid also in the case when some variation of the Hamiltonian $H \to H+V$, being of the "ordering" type, can be compensated by the introduction of the positive term $+\Delta(V)NS^2$; $\Delta(V) > 0$ for $V \neq 0$.

THEOREM 1B. If for the variation of the Hamiltonian $H \to H+W$ there exists a finite value of the parameter $\Delta = \Delta(W) > 0$ such that the condition (41) is valid (in particular, it is sufficient to suppose that the condition (42) is valid), then formulas (43),(43a) and (44) hold true (the last one in the case (42) only).

Note that for a large class of Hamiltonians the conditions of Theorem 1B are satisfied, if for $H+W/\theta_c$ one chooses the initial system for $\theta > \theta_c$, i.e., the system $H/\theta_c(1+\varepsilon)$, $\varepsilon > 0$.

9. Remarks on the Critical-Point Conditions

Let us consider the relations between different representations of the critical-point condition (16) (with respect to the concrete choice of δH).

Note first of all, that the basic condition in (16) is (16b), while (16a) is the auxiliary one. On the other hand, if one knows from the very beginning that the system H/θ_c is critical, then one can conclude that every (or "almost every") variation which satisfies (16a), satisfies also (16b)[14]. Indeed, let some fixed variation δH_0 satisfy (16a) and (16b) and, hence, the basic formula (31) be valid. Consider a set of different variations $\delta H = \delta H_1, \delta H_2, \ldots$, every one satisfing the condition (16a). Suppose, on the other hand, that the susceptibility $\chi[H+\rho NS^2/\theta_c] = 1/2\rho$ (31) is "stable" with respect to the variations δH_1, δH_2, ... and simultaneous variation (engaging) of the external field $-hNS$, i.e.,suppose that the following relation holds true

$$\lim_{\substack{\delta H_i \to 0 \\ h \to 0}} \chi\left[H+\rho NS^2+\delta H_i - h\,NS/\theta_c\right] \equiv \chi\left[\frac{H+\rho NS^2}{\theta_c}\right] = \frac{1}{2\rho}, \tag{45}$$

$$0 \le |h| \le 2\rho\left|S[H+\delta H_i/\theta_c]\right|, \quad i = 1,2,3,\ldots \tag{45a}$$

[14] We consider in this section the conditions (16) as restrictions on the possible choice of the variation δH.

independently of the "trajectory on the $\delta H_i - h$ -plane" when $\delta H_i \to 0$, $h \to 0$ (the parameter h varying in the region (45a)). Then one can insist that every variation δH_i which satisfies (16a) and (45) should satisfy also the basic condition (16b). To get this end, one should consider simultaneously the relation (45) and equality (30) (for $\delta H = \delta H_1$, δH_2, δH_3 ,....), which is valid owing to (16a) only. Then, as a result one gets (cf. (16b)):

$$\lim_{\delta H_i \to 0} \frac{S[H+\delta H_i + \rho N S^2/\theta_c]}{S[H+\delta H_i/\theta_c]} = 0, \quad i=1,2,\dots \qquad (46)$$

Consider now a special case when the variations are of the form

$$\delta H_i = -\xi_i N A_i \ , \quad i = 1,2,3,\dots \ , \qquad (47)$$

where A_i are fixed operators, ξ_i are small parameters, $\xi_i \to 0$. Then by analogy of the form (17) to (16b), one can rewrite (46) as [15]:

$$\frac{\chi_{SA_i}[H+\rho N S^2/\theta_c]}{\chi_{SA_i}[H/\theta_c]} = 0, \quad i = 1,2,\dots , \qquad (48)$$

where the "combined" susceptibility χ_{SA} for arbitrary system Γ/θ is definite as .

$$\chi_{SA}[\Gamma/\theta] = \{dS[\Gamma - \xi N A/\theta]/d\xi\}_{\xi\to 0},$$
$$\chi_{SA}[\Gamma/\theta] = \chi_{AS}[\Gamma/\theta]. \qquad (48a)$$

15) In this connection see also footnote 11.

So, we have obtained the following result:

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Let system H/θ_c be in the critical point with respect to the operator S in the sense of Def.1 (see (16)), and let a set of variations $\delta H = \delta H_1, \delta H_2, \ldots$ satisfy the conditions (16a) and (45). Then all these variations satisfy also (16b) (see (46)). If the variations mentioned are of the form (47), the condition (46) can be represented in the form (48).

The Lemma formulated makes it possible to elucidate the interrelation between different forms of the critical condition A - D (Section 5, (18), (20)-(22)). From the physical point of view the assumption (45) for the variations occuring in the conditions A-D seems to be natural. With this assumption, one can insist that if the condition (21) (all the more (22)) is satisfied, then (18b) follows from (18a) and (19b) follows from (19a). And if the conditions (18a) and (19a) are both valid, then if any of the two conditions (18b) and (19b) is satisfied, the second one is also valid.

APPENDIX A

Let us reproduce the fundamental theorem on the free energies due to N.N.Bogolubov, Jr. proved in ref.[6] (see also[7,8]). We choose here the form, which is convenient for our needs.

<u>THEOREM</u> (N.N.Bogolubov, Jr., 1966):

Consider an equilibrium system of N interacting particles with Hamiltonian Γ and temperature Θ (N is proportional to the volume of the system V). Let S_α ($\alpha = 1,2,\ldots,\tau$) be some operator constructions (not necessarily hermitian), which should satisfy the restrictions:

(A1a) $\| S_\alpha \| \leq K_1,$

(A1b) $\| S_\alpha \Gamma - \Gamma S_\alpha \| \leq K_2,$

(A1c)
$$\| S_\alpha S_\beta - S_\beta S_\alpha \| \leq K_3/N, \quad \| S_\alpha S_\beta^+ - S_\beta^+ S_\alpha \| \leq K_3/N,$$
$$\alpha, \beta = 1, 2, \ldots, \tau,$$

where $\| \dots \|$ means the norm of the operator, K_1, K_2, K_3 are constants.

Introduce the Hamiltonian:

$$\Gamma_\rho(C) = \Gamma + N \sum_{\alpha=1}^{r} \rho_\alpha (S_\alpha - C_\alpha)(S_\alpha^+ - C_\alpha^*), \quad (A2)$$

where ρ_α are positive parameters, $\rho_\alpha > 0$, C_α are complex variational parameters, varying in the region $|C_\alpha| \leq K_1 + \ell_1$, where ℓ_1 is an arbitrary small positive fixed number, $\ell_1 > 0$.

Introduce also the Hamiltonian with small "source" terms:

$$\Gamma_\nu = \Gamma - N \sum_{\alpha=1}^{r} (\nu_\alpha S_\alpha^+ + \nu_\alpha^* S_\alpha), \quad (A3)$$

where $0 \leq |\nu_\alpha| \leq \ell_2$, $\alpha = 1, 2, 3, \dots, r$, $\ell_2 > 0$ is arbitrary small positive fixed number.

Systems with the Hamiltonians Γ_ν and $\Gamma_\rho(C)$ are supposed to be thermodynamically stable for given fixed temperature $\theta \geq 0$[16], so that the corresponding free energies and canonical averages of the operators S_α exist both for finite N and in the limit $N \to \infty$[17].

Then in the limit $N \to \infty$ the following bounds hold true:

$$0 \leq \text{abs} \min_C f_N[\Gamma_\rho(C)] - f_N[\Gamma] \leq \varepsilon_N, \; \varepsilon_N \sim N^{-2/5} \xrightarrow[N \to \infty]{} 0, \quad (A4)$$

CONSEQUENCE: If one calculates first

$$f_\infty[H_\rho(C)] = \lim_{N \to \infty} f_N[H_\rho(C)], \quad (A5)$$

and then determines parameters C_α from the condition of the absolute minimum of the expression thus obtained: $C_\alpha = \overline{C}_\alpha$, where

$$f_\infty[\Gamma_\rho(\overline{C})] = \text{abs} \min_C f_\infty[\Gamma_\rho(C)], \quad (A6)$$

then the following bounds are valid [7,8]:

$$0 \leq \sum_{\alpha=1}^{r} \rho_\alpha \langle (S_\alpha - \overline{C}_\alpha)(S_\alpha^+ - \overline{C}_\alpha^*) \rangle_{\Gamma_\rho(\overline{C})} \leq \quad (A7)$$

$$\leq f_\infty[\Gamma_\rho(\overline{C})] - f_N[\Gamma] \leq \varepsilon_N + \eta_N, \; \varepsilon_N \to 0, \; \eta_N \to 0 \text{ as } N \to \infty,$$

$$\eta_N = \max_C |f_N[\Gamma_\rho(C)] - f_\infty[\Gamma_\rho(C)]|. \quad (A7a)$$

---

[16] Here and below the temperature is supposed to be fixed and is not indicated explicitly.

[17] By $N \to \infty$ we mean the thermodynamical limit, see footnote 5.

On the basis of (A6) and (A7) one can easily find that parameters $\overline{C}_\alpha$ are independent of $\rho_\alpha > 0$. On the other hand, in view of (A7) we have the relations:

$$\left|\overline{C}_\alpha - \langle S_\alpha \rangle_{\Gamma_\rho(\overline{C})}\right|^2 \leq (\varepsilon_N + \eta_N)/\rho_\alpha, \tag{A8a}$$

$$\left|\,|\overline{C}_\alpha|^2 - \langle S_\alpha S_\alpha^+ \rangle_{\Gamma_\rho(\overline{C})}\right| \leq (\varepsilon_N + \eta_N)/\rho_\alpha, \tag{A8b}$$
$$\alpha = 1, 2, \ldots, r.$$

Therefore

$$\overline{C}_\alpha = \lim_{N\to\infty} \langle S_\alpha \rangle_{\Gamma_\rho(\overline{C})}, \quad \overline{C}_\alpha^* = \lim_{N\to\infty} \langle S_\alpha^+ \rangle_{\Gamma_\rho(\overline{C})}, \tag{A8c}$$

$$|\overline{C}_\alpha|^2 = \lim_{N\to\infty} \langle S_\alpha S_\alpha^+ \rangle_{\Gamma_\rho(\overline{C})} \equiv \lim_{N\to\infty} \langle S_\alpha^+ S_\alpha \rangle_{\Gamma_\rho(\overline{C})}; \tag{A8d}$$
$$\rho_\alpha > 0, \quad \alpha = 1, 2, \ldots r.$$

where $\rho_\alpha > 0$ are arbitrary fixed values. Taking here the limit $\rho_\alpha \to 0$, we find that parameters $\overline{C}_\alpha$ appear to be the quasi-averages $\prec S_\alpha \succ_\Gamma$. Here $\Gamma_\rho(\overline{C})$ plays the role analogous to that of H_h in (7).

In our notation (section 4) a set of equations (A8c) can be rewritten in the form:

$$S_\alpha[\Gamma/\theta] = S_\alpha\Big[\Gamma + N\sum_{\alpha=1}^{r} \rho_\alpha S_\alpha S_\alpha^+ -$$
$$- N\sum_{\alpha=1}^{r} (\nu_\alpha S_\alpha^+ + \nu_\alpha^* S_\alpha)\Big]_{\nu_\alpha^\# = 2\rho_\alpha S_\alpha^\#[\Gamma/\theta]}, \tag{A9}$$
$$\alpha = 1, 2, \ldots, r.$$

Note also that owing to (A8d)

$$S_\alpha S_\alpha^+[\Gamma/\theta] \equiv S_\alpha^+ S_\alpha[\Gamma/\theta] = |S_\alpha[\Gamma/\theta]|^2, \quad \alpha = 1, 2, \ldots, r. \tag{A10}$$

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One can easily see, analysing the proof of the Theorem in refs. /6,8/ that the conditions (A1) can be chosen in a weakened form, when $\|Y\|$ in (A1) means not generally accepted (in the mathematical sense) norm of the operator Y, but the "average norm":

$$\| Y \| = \left(\frac{1}{2} \langle Y\overset{+}{Y} + \overset{+}{Y}Y \rangle_{\Gamma_D} \right)^{1/2}, \tag{A11}$$

where the averaging is taken over the Hamiltonian Γ_D (A4).

So, the Theorem and its consequences are valid also for unbounded (in the mathematical sense) operators. One has only to verify, making use of one or another additional consideration, that conditions (A1) with the"norm" of (A11) hold 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 September 28 1979.