

SELF-CONSISTENT FIELD METHOD FOR THE DESCRIPTION
OF PHASE TRANSITIONS

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Phase transitions in the Ising model and in crystals are considered for large interaction ranges r_0 . It is shown that the results of the phenomenological theory are valid over a broad temperature range. By successive application of the self-consistent field method, corrections to the thermodynamic quantities and correlation function have been found as a series in terms of r_0^{-3} . As the temperature approaches the transition temperature T_c , the parameter increases like $r_0^{-3}|T - T_c|^{-1/2}$ for finite-range forces and like $r^{-3} \ln |T - T_c|$ for dipole-dipole interactions in uniaxial ferroelectrics.

1. INTRODUCTION

It is known that Landau's phenomenological theory^[1] gives a satisfactory qualitative description of second-order phase transitions. In many cases, the temperature dependence that follows from this theory agrees with experiment over a wide temperature interval. However, this theory no longer holds in the direct vicinity of the transition point T_c . This is indicated both by the growth of the heat capacity at the transition point, observed experimentally in many cases,^[2] and by theoretical considerations concerning the growth of the fluctuations near T_c .^[3] In this paper we determine the region of applicability of the Landau theory.

From the microscopic point of view, the phenomenological theory is equivalent to the zero-order self-consistent-field approximation. This approximation is called the Curie-Weiss molecular field method, in the theory of ferromagnetism the Bragg-Williams method in the theory of binary alloys, and the Bardeen-Cooper-Schrieffer-Bogolyubov method in the theory of superconductivity. In ferroelectricity theory, this method was first used by Kurchatov.^[4] In this method, the field acting on an isolated particle and due to the remaining particles is replaced by an average field that does not depend on the position of the given particle, determined from the self-consistency conditions. It is obvious that this approximation is the better, the larger the ratio r_0 of the interaction radius to the average distance between particles and therefore the corrections to the zeroth self-consistent-field approximation contain reciprocal powers of r_0 (more accurately, of the interaction volume r_0^3). We present below a method for constructing such

expansions.

As the temperature T approaches T_c , the correlation in the particle position increases, so that even when r_0^3 is large the average-field approximation is no longer applicable. This is manifested formally in the fact that at small $\tau = |T - T_c|T_c^{-1}$ the expansion parameter becomes the quantity $r_0^{-3}\tau^{-1/2}$ (or $r_0^{-3} \ln \tau$, as in uniaxial ferroelectrics). The phenomenological theory starts from the expansion of the thermodynamic potential in powers of τ , i.e., it is applicable for small τ , therefore this theory is applicable only for sufficiently large r_0 in the temperature interval $r_0^{-6} \ll \tau \ll 1$ (or $\exp(-r_0^3) \ll \tau \ll 1$). Thus, for example, in the case of the Ising model with nearest-neighbor interaction, when $r_0 = 1$, there is no region of applicability of the thermodynamic theory, as is well known from the exact solution of this problem.^[1]

In Sec. 2 we consider the Ising model with arbitrary long-range potential. Using as an example this simplest model (which is used, as is well known, for the description of phase transitions in binary alloys and at the critical point), we shall illustrate the method of constructing the successive approximation—the series in powers of r_0^{-3} . Two first terms of the expansion in this parameter are obtained in the correlation function and in the thermodynamic quantities.

In Sec. 3 the developed methods are applied to the more complicated case of phase transitions in which the crystal symmetry changes. In Sec. 4 we consider the influence of the electric dipole-dipole interaction in ferroelectrics, which leads to an extension of the region of applicability of the phenomenological theory and to a decrease in the required

corrections. In Sec. 5, finally, we consider the question of the phase transitions in one-dimensional systems.

We note that the effects of the first correction term of the thermodynamic theory were discussed phenomenologically in earlier papers by Levanyuk^[5, 6] and also by I. M. Lifshitz. The present article supplements these papers in that it starts from a microscopic analysis and indicates both the region of applicability and the method of constructing the next higher approximations.

2. ISING MODEL WITH LONG-RANGE ACTION

Let us consider the simplest model of the Ising type, constituting a lattice of dipoles, each of which assumes only two positions, with Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{\mathbf{r} \neq \mathbf{r}'} V_{\mathbf{r}-\mathbf{r}'} \sigma_{\mathbf{r}} \sigma_{\mathbf{r}'} - H \sum_{\mathbf{r}} \sigma_{\mathbf{r}}. \quad (1)$$

Here $\sigma_{\mathbf{r}} = \pm 1$, \mathbf{r} is the coordinate of the cell site, H the external magnetic field, and the potential $V_{\mathbf{r}-\mathbf{r}'}$ has a large action radius r_0 . To construct the successive self-consistent field approximations it is convenient to isolate in (1) the interaction with average spin $s = \langle \sigma \rangle$. The partition function Z then takes the form

$$Z = \text{Sp} \exp \left[-N\beta V_0 s^2 / 2 + \beta \sum_{\mathbf{r}} \sigma_{\mathbf{r}} (V_0 s + H) + \frac{1}{2} \beta \sum_{\mathbf{r} \neq \mathbf{r}'} V_{\mathbf{r}-\mathbf{r}'} (\sigma_{\mathbf{r}} - s) (\sigma_{\mathbf{r}'} - s) \right],$$

$$\beta = 1/T, \quad V_0 = \sum_{\mathbf{r}} V_{\mathbf{r}}, \quad (2)$$

N is the number of sites.

The zeroth self-consistent field approximation is obtained by neglecting the last term in the exponential in (2). With this, the distribution function f breaks up into a product of functions for each cell:

$$f = \prod_{\mathbf{r}} f_0(\sigma_{\mathbf{r}}),$$

$$f_0 = (\text{Sp} \exp(\sigma y))^{-1} \exp \sigma y = \frac{1}{2} (1 + \sigma \text{th } y),$$

$$y = \beta (V_0 s + H). \quad (3)^*$$

The free energy per cell F is given by

$$\beta F^{(0)} = \beta V_0 s^2 / 2 - \ln \text{ch } \beta (V_0 s + H)$$

$$= (y - \beta H)^2 / 2\beta V_0 - \ln \text{ch } y, \quad (4)^\dagger$$

and the value of s can be obtained either by averaging σ over the distribution function (3), or from the condition of the minimum of the free energy, $\partial F / \partial s = 0$:

$$s = \text{th } \beta (V_0 s + H). \quad (5)$$

Formulas (4) and (5) are exact for that (unphysical) case when each particle interacts with all the remaining ones with potential $V_0 N^{-1}$.^[7] From (4) and (5) we obtain the known results of the phenomenological theory. In the absence of a magnetic field, a second-order phase transition takes place in the system at a temperature $T_C = V_0$. $s = 0$ above the transition, and below it there appears a spontaneous moment that varies near the transition like $s^2 = 3\tau$. The heat capacity at $T > T_C$ is equal to zero, and at the transition point it experiences a discontinuity $C_- - C_+ = 3/2$. The susceptibility $\chi = \partial s / \partial H |_{H=0}$ increases near T_C in accord with the Curie-Weiss law: $\chi_+ = (T_C \tau)^{-1}$ for $T > T_C$ and $\chi_- = (2T_C \tau)^{-1}$ for $T < T_C$.

The foregoing approximation is equivalent to replacing the spins interacting with the given spin by their mean values. The last term in (2), which describes the influence of the deviations of the field from the mean value, constitutes at large values of r_0 a small quantity, in powers of which the expansion will be carried out. In each approximation it is necessary to take into account also the corrections to the mean value of the spin, i.e., to the "zeroth" terms in the exponential of (2). It is physically obvious that the average spin, which is a free parameter of the system, minimizes the free energy F , and it is therefore simplest to find s from the equation $\partial F / \partial s = 0$ or $\partial F / \partial y = 0$, where y is defined in (3). It can be shown that this equation coincides with the self-consistency equation $s = \langle \sigma \rangle$.

We shall find useful in what follows the following exact relation between the free energy and the correlation function. If we introduce formally the factor g preceding the last term in the exponential of (2), then the free energy will be a function of g , with $g = 1$ corresponding to the real case. Then we have for the derivative $\partial F / \partial g$, taking into account the fact that $\partial F / \partial y = 0$,

$$-\frac{\partial F}{\partial g} = \frac{1}{2N} \sum_{\mathbf{r} \neq \mathbf{r}'} V_{\mathbf{r}-\mathbf{r}'} \langle \sigma_{\mathbf{r}} - s, \sigma_{\mathbf{r}'} - s \rangle = \frac{1}{2} \sum_{\mathbf{k}} V_{\mathbf{k}} K_{\mathbf{k}}, \quad (6)$$

where $V_{\mathbf{k}}$ and $K_{\mathbf{k}}$ are the Fourier components of the potential and of the correlation function:

$$V_{\mathbf{k}} = \sum_{\mathbf{r}} V_{\mathbf{r}} \exp(-i\mathbf{k}\mathbf{r}),$$

$$K_{\mathbf{k}} = \sum_{\mathbf{r}} \exp(i\mathbf{k}(\mathbf{r}-\mathbf{r}')) \langle \sigma_{\mathbf{r}} - s, \sigma_{\mathbf{r}'} - s \rangle. \quad (7)$$

*th \equiv tanh.

†ch \equiv cosh.

The first correction to the zeroth approximation, which takes into account the correlation of the particles, can be found by a method analogous to the well-known Debye approximation in the theory of ionized gases.^[8] The expression (6) can be re-written in the form

$$\frac{1}{2N} \sum_{\mathbf{r}'} \left\langle (\sigma_{\mathbf{r}'} - s) \sum_{\mathbf{r} \neq \mathbf{r}'} V_{\mathbf{r}-\mathbf{r}'} \langle \sigma_{\mathbf{r}} - s \rangle' \right\rangle = \frac{1}{2N} \sum_{\mathbf{r}'} \langle \sigma_{\mathbf{r}'} - s \rangle h_0, \quad (8)$$

where the averaging $\langle \dots \rangle'$ is carried out at fixed $\sigma_{\mathbf{r}'}$, and the quantity $h_{\mathbf{r}-\mathbf{r}'}$, equal to

$$\begin{aligned} h_{\mathbf{r}-\mathbf{r}'} &= \sum_{\mathbf{r}''} V_{\mathbf{r}-\mathbf{r}''} \langle \sigma_{\mathbf{r}''} - s \rangle' = V_{\mathbf{r}-\mathbf{r}'} (\sigma_{\mathbf{r}'} - s) \\ &+ \sum_{\mathbf{r}'' \neq \mathbf{r}'} V_{\mathbf{r}-\mathbf{r}''} \langle (\sigma_{\mathbf{r}''} - s) \exp \left\{ \beta (\sigma_{\mathbf{r}''} - s) g \sum_{\mathbf{p}} V_{\mathbf{r}''-\mathbf{p}} (\sigma_{\mathbf{p}} - s) \right\} \\ &\times f_0 (\sigma_{\mathbf{r}''}) \rangle', \end{aligned} \quad (9)$$

has the meaning of the average field in the cell \mathbf{r} , produced following a specified deviation of $\sigma_{\mathbf{r}'}$, from s . The last term of (9) contains explicitly the factors containing $\sigma_{\mathbf{r}''}$, and the remaining are included under the averaging sign. The exponential in (9) contains the sum of a large number of terms, with a mean value $h_{\mathbf{r}''-\mathbf{r}'}$. Taking into account the smallness of this quantity and again neglecting the fluctuations, we arrive at an expression for h :

$$h_{\mathbf{r}-\mathbf{r}'} = V_{\mathbf{r}-\mathbf{r}'} (\sigma_{\mathbf{r}'} - s) + \beta g \sum_{\mathbf{r}''} V_{\mathbf{r}-\mathbf{r}''} h_{\mathbf{r}''-\mathbf{r}'} \langle (\sigma_{\mathbf{r}''} - s)^2 \rangle. \quad (10)$$

The mean value in the last term is taken already over f_0 , giving the quantity $\cosh^{-2} y$, which does not depend on \mathbf{r}'' . Solving (10) with the aid of a Fourier transformation, we obtain for $h_{\mathbf{k}}$ the expression $V_{\mathbf{k}} (\sigma_{\mathbf{r}'} - s) \times (1 - g\beta V_{\mathbf{k}} \cosh^{-2} y)^{-1}$. Using (8) and (6), we obtain hence for the correlation function $K_{\mathbf{k}}$ ($g = 1$)

$$\begin{aligned} K_{\mathbf{k}} &= \langle (\sigma - s)^2 \rangle (1 - \beta V_{\mathbf{k}} \langle (\sigma - s)^2 \rangle)^{-1} \\ &= \cosh^{-2} y (1 - \beta V_{\mathbf{k}} \cosh^{-2} y)^{-1}. \end{aligned} \quad (11)$$

We shall consider potentials $V_{\mathbf{r}}$ whose Fourier component $V_{\mathbf{k}}$ reach a maximum at $k = 0$, as is the case, say, for an attraction potential that does not reverse sign. We assume also that $V_{\mathbf{r}}$ is spherically symmetrical, and its rms radius, defined by

$$r_0^2 = \frac{\sum_{\mathbf{r}} r^2 V_{\mathbf{r}}}{\sum_{\mathbf{r}} V_{\mathbf{r}}}, \quad (12)$$

is large but finite. The case of infinite r_0 (dipole-dipole interaction) is considered in Sec. 4. Then the expansion of $V_{\mathbf{k}}$ in small k is of the form $V_{\mathbf{k}} = V_0 (1 - k^2 r_0^2 / 6)$, and near the transition point, for small H , τ , and $kr_0 \ll 1$, the correlation function behaves, in accordance with (11), like

$$K_{\mathbf{k}} = (u + k^2 r_0^2 / 6)^{-1}, \quad u = y^2 + (T - T_c) T_c^{-1}. \quad (13)$$

In the absence of a magnetic field $u = \tau$ for $T > T_c$ and $u = 2\tau$ for $T < T_c$. Expression (13) coincides in form with the Ornstein-Zernike correlation function.^[9] For small τ , the correlation radius increases like $r_0 \tau^{-1/2}$, and at the transition point the correlations decrease in power-law fashion.

For the free energy F we have, taking (11) and (6) into account

$$\begin{aligned} \beta F &= \beta F^{(0)} + \frac{1}{2} \sum_{\mathbf{k}} \ln(1 - \beta V_{\mathbf{k}} \cosh^{-2} y) \\ &= \frac{(y - \beta H)^2}{2\beta V_0} - \ln \cosh y + \frac{1}{2} \sum_{\mathbf{k}} \ln(1 - \beta V_{\mathbf{k}} \cosh^{-2} y). \end{aligned} \quad (14)$$

The equation for the average spin is obtained by equating $\partial F / \partial y$ to zero:

$$s = \frac{y - \beta H}{\beta V_0} = \text{th } y \left(1 - \sum_{\mathbf{k}} \frac{\beta V_{\mathbf{k}} \cosh^{-2} y}{1 - \beta V_{\mathbf{k}} \cosh^{-2} y} \right). \quad (15)$$

The susceptibility in the magnetic field, $\chi_H = \partial s / \partial H$, can be obtained from (15):

$$\chi_H = \frac{\beta \Pi}{1 - \beta V_0 \Pi},$$

$$\begin{aligned} \Pi &= \cosh^{-2} y - \cosh^{-2} y (1 - 2 \text{sh}^2 y) \sum_{\mathbf{q}} \frac{\alpha_{\mathbf{q}}}{1 - \alpha_{\mathbf{q}}} \\ &+ 2 \text{th}^2 y \sum_{\mathbf{q}} \frac{\alpha_{\mathbf{q}}^2}{(1 - \alpha_{\mathbf{q}})^2} \quad \alpha_{\mathbf{q}} = \beta V_{\mathbf{q}} \cosh^{-2} y. \end{aligned} \quad (16)^*$$

In this approximation, the transition point is determined from (13) with $H = 0$ and $y \rightarrow 0$:

$$T_c = V_0 \left(1 - \sum_{\mathbf{q}} \frac{V_{\mathbf{q}}}{V_0 - V_{\mathbf{q}}} \right). \quad (17)$$

The expression for the different thermodynamic quantities can be obtained from (14)–(16) by expanding in powers of H and τ . Taking into account the zero-order approximation term, we obtain

$$\begin{aligned} s^2 &= 3\tau \left(1 + \alpha \sqrt{\frac{2}{\tau}} \right), \quad C_+ = \frac{\alpha}{4\sqrt{\tau}}, \quad C_- = \frac{3}{2} + \frac{\alpha}{\sqrt{2\tau}}, \\ \chi_+^{-1} &= T_c \tau \left(1 - \frac{\alpha}{\sqrt{\tau}} \right), \quad \chi_-^{-1} = 2T_c \tau \left(1 + \frac{\alpha}{2\sqrt{2\tau}} \right), \\ \alpha &= \frac{3\sqrt{6}}{2\pi r_0^3}. \end{aligned} \quad (18)$$

*sh \equiv sinh.

We have left out from (18) all terms proportional to α , and also those proportional to τ and obtained by expanding the "zero-order" expressions (4) and (5). From (18) follows the statement made above that the corrections to the results of the phenomenological theory have a relative order $r_0^{-3}\tau^{-1/2}$. These formulas are valid so long as the correction is small, i.e., when $\alpha \ll \sqrt{\tau}$.

To calculate the next higher approximations, and also to obtain a more rigorous justification of the foregoing intuitive method, it is convenient to make use of the already developed diagram methods. We introduce in lieu of the quantities $\sigma_{\mathbf{r}}$ the Fermi operators $a_{\mathbf{r}}$ and $a_{\mathbf{r}}^+$, using the relations

$$\sigma_{\mathbf{r}} = 2a_{\mathbf{r}}^+a_{\mathbf{r}} - 1, \quad \{a_{\mathbf{r}}, a_{\mathbf{r}'}^+\} = \delta_{\mathbf{r}\mathbf{r}}. \quad (19)$$

The Hamiltonian (1) assumes the usual four-fermion form, without the kinetic energy, and the magnetic field plays the role of the chemical potential. In the case under consideration, that of large r_0 , the Fourier component of the potential $V_{\mathbf{k}}$ is large for small \mathbf{k} , and decreases rapidly when $kr_0 \gg 1$. Therefore the resultant problem is similar to the problem of the thermodynamic functions of a plasma,^[10] where a similar isolation was carried out of the long-range effects. The cited article contains a method of successive self-consistent-field approximation method, which we shall employ.

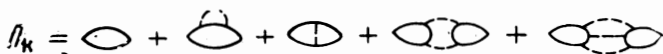
We write the correlation function (7) in the form (see, e.g.,^[11])

$$K_{\mathbf{k}}(g) = \frac{\Pi_{\mathbf{k}}}{1 - \beta g V_{\mathbf{k}} \Pi_{\mathbf{k}}}, \quad (20)$$

where the irreducible part $\Pi_{\mathbf{k}}$ does not contain single lines of the potential $V_{\mathbf{k}}$. In calculating $\Pi_{\mathbf{k}}$ we can already expand in powers of the interaction, since the factors $V_{\mathbf{q}}$ contained in it are integrated with respect to \mathbf{q} , which leads to the reciprocal powers of r_0^{-3} . The first terms of the expansion of $\Pi_{\mathbf{k}}$ are shown graphically in the figure. The dashed line corresponds to an effective interaction $V_{\mathbf{k}}(1 - \beta g V_{\mathbf{k}} \Pi_{\mathbf{k}})^{-1}$, and the solid line to the "zeroth" fermion Green's function $G^0(\mathbf{r}, \tau)$ (here and in (21) τ is the "imaginary time" of the temperature diagram technique^[12]).

In the absence of a magnetic field above the transition the fermion density is $n = \langle a_{\mathbf{r}}^+ a_{\mathbf{r}} \rangle = 1/2 = 1 - n$, and below the transition $n = 1/2(1 + \tanh y)$, and the symmetry of the "particles" and "holes" is lost.

The zeroth approximation for $\Pi_{\mathbf{k}}$ is given by the first diagram of the figure:



$$\begin{aligned} \Pi_{\mathbf{k}}^{(0)} &= -4 \sum_{\mathbf{r}} G^0(\mathbf{r}, \tau) G^0(-\mathbf{r}, -\tau) e^{i\mathbf{k}\mathbf{r}} \\ &= 4n(1 - n) = \text{ch}^{-2}y. \end{aligned} \quad (21)$$

Comparing (20) and (21) with (11) we verify that the Debye approximation corresponds to the zeroth approximation in $\Pi_{\mathbf{k}}$.^[10]

In the next approximation for $\Pi_{\mathbf{k}}$, it is necessary to take into account diagrams with one and two internal dashed lines. The calculation can be carried out in standard fashion; it is simpler, however, to use the first-approximation formula (16) for the susceptibility in the magnetic field. From the definition $\chi_{\mathbf{H}} = \partial \langle \sigma \rangle / \partial \mathbf{H}$ can be readily seen that $\chi_{\mathbf{H}}$ coincides with the values of the correlation function $K_{\mathbf{k}}$ (7) for $\mathbf{k} = 0$. Therefore the quantity Π in (16) is the value of the irreducible part of $\Pi_{\mathbf{k}}$ of formula (2) with $\mathbf{k} = 0$ (and $g = 1$). From the form of the first-approximation diagrams for $\Pi_{\mathbf{k}}$ we can easily reconstruct from this particular value the total function $\Pi_{\mathbf{k}}(g)$:

$$\begin{aligned} \Pi_{\mathbf{k}}(g) &= \text{ch}^{-2}y - \text{ch}^{-2}y(1 - 2\text{sh}^2y) \sum_{\mathbf{q}} \frac{g\alpha_{\mathbf{q}}}{1 - g\alpha_{\mathbf{q}}} \\ &+ 2\text{th}^2y \sum_{\mathbf{q}} \frac{g\alpha_{\mathbf{q}}}{1 - g\alpha_{\mathbf{q}}} \frac{g\alpha_{\mathbf{k}-\mathbf{q}}}{1 - g\alpha_{\mathbf{k}-\mathbf{q}}}. \end{aligned} \quad (22)$$

From (22) and (20) we obtain for the correlation function near the transition

$$K_{\mathbf{k}}^{-1} = u + k^2r_0^2/6 - \alpha\sqrt{u} - (2\alpha y^2\sqrt{6}/kr_0) \text{arc tg}(kr_0/2\sqrt{6}u), \quad (23)$$

where u is the same as in (13). In the absence of a magnetic field, taking into account expression (18) for s^2 , we have

$$T > T_c: K_{\mathbf{k}}^{-1} = k^2r_0^2/6 + \tau - \alpha\sqrt{\tau},$$

$$T < T_c:$$

$$K_{\mathbf{k}}^{-1} = \frac{k^2r_0^2}{6} + 2\tau + 2\alpha\sqrt{2\tau} - \left(\frac{6\alpha\tau\sqrt{6}}{kr_0} \right) \tan^{-1}\left(\frac{kr_0}{4\sqrt{3\tau}} \right). \quad (24)$$

We note that the corrections to $K_{\mathbf{k}}$ have a relative order of magnitude $\alpha\tau^{-1/2}$ when $kr_0 < \sqrt{\tau}$ and $\alpha\sqrt{\tau}(kr_0)^{-2}$ when $kr_0 > \sqrt{\tau}$.

With the aid of (22), (20), and (6) we obtain an expression for the free energy with second-approximation corrections:

$$\begin{aligned} \beta F &= \frac{(y - \beta H)^2}{2\beta V_0} - \ln \text{ch } y \\ &+ \frac{1}{2} \int_0^{\beta \text{ch}^{-2}y} d\xi \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}}{1 - \xi V_{\mathbf{k}} + \xi^2 V_{\mathbf{k}} \sum_{\mathbf{q}} V_{\mathbf{q}}(1 - \xi V_{\mathbf{q}})^{-1}} \end{aligned}$$

$$-\frac{\text{sh}^2 y}{2} \left(\sum_q \frac{\alpha_q}{1 - \alpha_q} \right)^2 - \frac{\text{sh}^2 y}{3} \sum_{k, q} \frac{\alpha_q}{1 - \alpha_q} \frac{\alpha_k}{1 - \alpha_k} \frac{\alpha_{k+q}}{1 - \alpha_{k+q}}. \quad (25)$$

Here α_q is given by formula (16). In the third term of (25) it would be necessary, strictly speaking, to expand the denominator up to first order in the ratio of the last term to the first two, as was done to obtain the last terms in (25). However, the renormalization of T_c given by (17) is more simply taken into account with the chosen notation.

The equation for the average moment is obtained by equating to zero the derivative of (25) with respect to y , and an equation similar to (16) is obtained for χ_H by differentiating with respect to H the equation for the moment. The general formulas, however, become cumbersome, and we therefore confine ourselves to the region near the transition. The contribution of the fourth term in (25) is small here and can be discarded, and in the last integral the small quantities k and $q < r_0^{-1}$ are significant only in logarithmic accuracy, so that calculation of the factor under the logarithm sign calls for knowledge of $V_{\mathbf{r}}$ also in the region $r \sim r_0$. If we assume, for example, a simple exponential form $V_{\mathbf{r}} = \text{const} \exp(-rr_0^{-1}\sqrt{12})$ for $V_{\mathbf{r}}$ at $r \gtrsim r_0$, then the integral can be easily calculated by going over to the coordinate representation. As a result, the equation for the moment takes the form

$$y^3 - 3HT_c^{-1} = 3y \left[\frac{T_c - T}{T_c} + \alpha \sqrt{u} - \frac{\alpha^2}{2} - \frac{\alpha^2}{3} (\ln(16u) + y^2/u) \right], \quad (26)$$

where, as above, $u = y^2 + (T - T_c)T_c^{-1}$. We retain here the symbol T_c as defined by (17), for owing to the presence of the logarithmic term in (26) we cannot introduce formally a "new" temperature of transition as the point where the square bracket vanishes at $H = 0$ and $y \rightarrow 0$.

Using (25) and (26), as well as the formula for s^2 from the preceding approximation, we obtain in lieu of (18)

$$s^2 = 3\tau \left[1 + \alpha \sqrt{\frac{2}{\tau}} + \frac{\alpha^2}{2\tau} - \frac{\alpha^2}{3\tau} \ln 32\tau \right],$$

$$C_- = \frac{3}{2} + \frac{\alpha}{\sqrt{2}\tau} - \frac{\alpha^2}{2\tau},$$

$$C_+ = \frac{\alpha}{4\sqrt{\tau}} + \frac{\alpha^3}{12\tau^{3/2}} \left[\ln \frac{1}{\tau} - 2 \ln \frac{16}{3} + 2 \right],$$

$$\chi_+^{-1} = T_c \tau \left[1 - \frac{\alpha}{\sqrt{\tau}} + \frac{\alpha^2}{2\tau} - \frac{\alpha^2}{3\tau} \ln \frac{1}{16\tau} \right],$$

$$\chi_-^{-1} = 2T_c \tau \left[1 + \frac{\alpha}{\sqrt{8\tau}} + \frac{3\alpha^2}{8\tau} - \frac{\alpha^2}{3\tau} \ln 32\tau \right]. \quad (27)$$

In the expression for the heat capacity C_+ above the transition, the second-order terms α^2/τ cancel out, and we have therefore presented for it also the correction for the third-approximation, corresponding to the last diagram of the figure.

3. TRANSITIONS WITH CHANGE OF CRYSTAL SYMMETRY

Application of the foregoing method to real systems calls for an analysis of concrete models. However, the results are insensitive to the type of model, so that we shall consider for simplicity the following model:^[13] Let an isolated atom of the cell move in a field $u(\mathbf{r})$ having tetragonal symmetry and produced by atoms of a different species, and let it interact with a potential $-V_{ij}(\mathbf{r}_i, \mathbf{r}_j) = -(\mathbf{r}_i \cdot \mathbf{r}_j)V_\rho$ with the atoms of the other cells (ρ = distance between cells i and j). The phase transition consists in the fact that at $T < T_c$ the cell loses the symmetry center as a result of the appearance of an average displacement $\langle \mathbf{r} \rangle = \mathbf{s}$ from the center. Assume, furthermore, the presence of an external electric field \mathbf{E} , with a potential proportional to the displacement of the atom \mathbf{r}_i . Denoting that part of the free energy which is regular near T_c by F_0 , we have

$$-\beta(F - F_0)N = \ln \int \exp \left[-\beta \sum_i u(\mathbf{r}_i) + \beta e_{\text{eff}} \mathbf{E} \sum_i \mathbf{r}_i + \frac{\beta}{2} \sum_{i \neq j} (\mathbf{r}_i \mathbf{r}_j) V_\rho \right] \prod_i d\mathbf{r}_i. \quad (28)$$

Introducing the vector $\mathbf{y} = \beta(V_0 \mathbf{s} + e_{\text{eff}} \mathbf{E})$, analogous to the y introduced in (3), we obtain zero-order equations similar to (4) and (5) for the free energy and the average displacement:

$$\beta(F - F_0) = (\mathbf{y} - \beta e_{\text{eff}} \mathbf{E})^2 / 2\beta V_0 - \ln \int \exp[-\beta u(\mathbf{r}) + \mathbf{r}\mathbf{y}] d\mathbf{r},$$

$$\mathbf{s} = (\mathbf{y} - \beta e_{\text{eff}} \mathbf{E}) / \beta V_0 = \int \mathbf{r} \exp[-\beta u(\mathbf{r}) + \mathbf{r}\mathbf{y}] d\mathbf{r}. \quad (29)$$

When $\mathbf{E} = 0$ and $V_0 > 0$, a phase transition takes place in the system at a temperature determined by the second equation of (29) as $y \rightarrow 0$:

$$1) \Pi_{\parallel} > \Pi_{\perp}: \quad T_c = T_{c\parallel} = V_0 \Pi_{\parallel};$$

$$2) \Pi_{\parallel} < \Pi_{\perp}: \quad T_c = T_{c\perp} = V_0 \Pi_{\perp};$$

$$\Pi_{\parallel} = \overline{x^2} = \int x^2 n_0(\mathbf{r}) d\mathbf{r},$$

$$\begin{aligned} \Pi_{\perp} &= \overline{y^2} = \overline{z^2} = \int z^2 n_0(\mathbf{r}) d\mathbf{r}, \\ n_0 &= e^{-\beta_c u(\mathbf{r})} \left(\int e^{-\beta_c u(\mathbf{r})} d\mathbf{r} \right)^{-1}. \end{aligned} \quad (30)$$

If the distribution of the atom in the cell is stretched along the x axis, $x^2 > y^2$, then, as the temperature is lowered, T_{CX} is reached first and the atom is displaced during the transition along the x axis; in the opposite case, the transition takes place at $T_{\text{C}\perp}$ and the atom is displaced in the yz plane; we consider for simplicity the first case. The singularities of the thermodynamic quantities have the same form as in the zeroth approximation of the Ising model. We assume with this also the satisfaction of the condition that the transition be of second order—the condition that the coefficient of y^4 in the expansion of $F^{(0)}$ in (29) in powers of y be positive, viz.: $3(\overline{x^2})^2 > \overline{x^4}$. Otherwise a first-order transition takes place in the system at a certain $T > T_{\text{CX}}$.

Introducing, in analogy with (7) and (6), the correlation functions $K_{\alpha\gamma}$ and the auxiliary charge g , describing the interaction via the components $V_{\mathbf{k}}$ with $\mathbf{k} \neq 0$, we obtain in lieu of (7) and (6)

$$\begin{aligned} K_{\alpha\gamma}(\rho_{ij}) &= \langle x_{\alpha}^i - s_{\alpha}, x_{\gamma}^j - s_{\gamma} \rangle, \\ K_{\alpha\gamma}(\mathbf{k}) &= \sum_{\rho} K_{\alpha\gamma}(\rho) \exp(ik\rho); \\ -\frac{\partial F}{\partial g} &= -\frac{1}{2} \sum_{\rho} \sum_{\alpha=1}^3 V_{\rho} K_{\alpha\alpha}(\rho) = \frac{1}{2} \sum_{\mathbf{k}, \alpha} V_{\mathbf{k}} K_{\alpha\alpha}(\mathbf{k}). \end{aligned} \quad (31)$$

An equation for $K_{\alpha\gamma}$ similar to (11) is

$$\begin{aligned} K_{\alpha\gamma}(\mathbf{k}) &= \Pi_{\alpha\gamma} + \beta \sum_{\mu} \Pi_{\alpha\mu} V_{\mathbf{k}} K_{\mu\gamma}(\mathbf{k}), \Pi_{\alpha\gamma} \\ &= \frac{\partial s_{\alpha}}{\partial y_{\gamma}} = \langle x_{\alpha}^i - s_{\alpha}, x_{\gamma}^i - s_{\gamma} \rangle, \end{aligned} \quad (32)$$

where $\mathbf{s}(\mathbf{y})$ is given by (29). The correlation function that is singular near the transition is, in accord with (30), $K_{\text{XX}}(\mathbf{k}) = \Pi_{\text{XX}}(1 - \beta V_{\mathbf{k}} \Pi_{\text{XX}})^{-1}$. The correction to the free energy is given by a formula similar to (14):

$$\begin{aligned} \beta(F - F_0) &= \beta F^{(0)} + \sum_{\mathbf{k}} \ln(1 - \beta V_{\mathbf{k}} \Pi_{yy}) \\ &+ \frac{1}{2} \sum_{\mathbf{k}} \ln(1 - \beta V_{\mathbf{k}} \Pi_{xx}). \end{aligned} \quad (33)$$

Account is taken in the second term of the right-hand side of the fact that $\Pi_{yy} = \Pi_{zz}$; near T_{CX} this term is regular and can be included in F_0 .

Let the expansion of the potential $V_{\mathbf{k}}$ in small \mathbf{k} have the form $V_0(1 - k_x^2 x_0^2/2 - k_{\perp}^2 r_{\perp}^2/4)$, and let

the dependence of s_x in (29) on $y_x = y$ and τ near T_c be given by the expansion

$$s_x(y) = g_0 y \left(1 + g_1 \frac{T - T_c}{T_c} - g_2 \frac{y^2}{3} \right), \quad (34)$$

where $g_1 < 1$, and the constants g_0 and g_2 are positive and are connected with the corresponding constants of the Landau theory^[11] by the relations $a = (1 - g_1)/2g_0$, $C = g_2 T_c/12g_0^3$, and $\eta = s_x$. Then we see from the foregoing formulas that the correlation function has, as before, the Ornstein-Zernike form (13), and the relation between the singular parts of the free energy of the crystal $F_{\text{CF}}^{\text{sf}}$ and the Ising model (14) $F_{\text{I}}^{\text{sf}}(y^2, \tau, \alpha)$ is

$$F_{\text{cr}}^{\text{sf}} = \frac{g_0}{g_2} F_{\text{I}}^{\text{sf}}(g_2 y^2, \tau(1 - g_1), \alpha_{\text{cr}}), \alpha_{\text{cr}} = \frac{g_2}{g_0} \frac{\sqrt{2}}{\pi x_0 r_{\perp}^2}. \quad (35)$$

Therefore the singularities of the thermodynamic quantities are given by formulas (18), in which the constants are redefined as in (35).

The next approximation can be obtained by the same method as used in the derivation of formulas (22)–(25) of the Ising model. For the uniaxial transition in question, relation (35) is retained also in the higher approximations. It can be shown that this remains valid also in the quantum analysis.

4. CRYSTALS WITH DIPOLE-DIPOLE INTERACTION

So far we have considered interatomic-interaction potentials V_{ρ} whose action radius was finite, albeit large. As noted by Krivoglaz^[14] and by Levanyuk,^[6] the presence of dipole-dipole interaction can alter the results appreciably. For simplicity we shall again consider the model (28) and assume that the displacement of the atom \mathbf{r}_i leads to formation of a dipole moment $e_{\text{eff}} \mathbf{r}_i$, so that the phase transition is ferroelectric. In the exponent of (28) there is added a term with corresponding dipole-dipole interaction. We shall assume the geometry of the sample to be such that the resultant static polarization \mathcal{P} is uniform over the volume. Then, taking into account the known expression for the field \mathbf{E}_d acting at the center of the cell,^[15] $\mathbf{E}_d = \langle \mathbf{E} \rangle + 4\pi \mathcal{P}/3$, where $\langle \mathbf{E} \rangle$ is average macroscopic field, and taking account also of the smallness of the displacements relative to the cell dimensions we find that when $\langle \mathbf{E} \rangle = 0$ the phase transition point is determined not by (30) but by

$$\begin{aligned} 1) \quad &1 = \beta \Pi_{\parallel} (V_0 + \lambda/3) \equiv \beta \Pi_{\parallel} W_0, \\ 2) \quad &1 = \beta \Pi_{\perp} W_0, \quad \lambda = 4\pi e_{\text{eff}}^2 / v_c, \end{aligned} \quad (36)$$

v_c is the volume of the cell. In (32) we add to the

potential $V_{\mathbf{k}}$ a term corresponding to dipole-dipole interaction, so that these equations take the form

$$K_{\alpha\gamma}(\mathbf{k}) = \Pi_{\alpha\gamma} + \beta \sum_{\mu,\nu} \Pi_{\alpha\mu} V_{\mu\nu}(\mathbf{k}) K_{\nu\gamma}(\mathbf{k});$$

$$V_{\mu\nu}(\mathbf{k}) = V_{\mathbf{k}} \delta_{\mu\nu} + e_{\text{eff}}^2 \sum_j \left(\frac{\partial^2}{\partial \rho_\mu^i \partial \rho_\nu^i} \frac{1}{|\rho_i - \rho_j|} \right) e^{i\mathbf{k}\rho_{ij}}. \quad (37)$$

In the essential region of small \mathbf{k} (large, however, compared with the reciprocal dimensions of the sample), the expression for $V_{\mu\nu}(\mathbf{k})$ can be written in the form

$$V_{\mu\nu}(\mathbf{k}) = (V_{\mathbf{k}} + \lambda/3) \delta_{\mu\nu} - \lambda n_\mu n_\nu \equiv W_{\mathbf{k}} \delta_{\mu\nu} - \lambda n_\mu n_\nu, \\ n_\mu = k_\mu / k. \quad (38)$$

The expansion of the last term used in (38) for small \mathbf{k} can be obtained by means of a standard method in solid-state physics^[15] by breaking up the sum over the cells into regions lying inside and outside a sphere of some large but microscopic radius R such that $1 \ll R \ll k^{-1}$. In summing inside the sphere, one can neglect the argument of the exponential, so that this sum is equal to zero, and in the external region the sum can be replaced by an integral.

Using (38) and (37), and choosing the x axis, as before, along the tetragonal axis and the y axis to lie in the (x, \mathbf{k}) plane, we find that the nonvanishing elements $K_{\alpha\beta}$ for $T > T_c$ are

$$K_{zz} = \Pi_{\perp} (1 - \beta W_{\mathbf{k}} \Pi_{\perp})^{-1}, \\ K_{xx} = \Pi_{\parallel} (1 - \beta W_{\mathbf{k}} \Pi_{\perp} + \beta \lambda n_y^2 \Pi_{\perp}) \Delta_{\mathbf{k}}^{-1}, \\ K_{yy} = \Pi_{\perp} (1 - \beta W_{\mathbf{k}} \Pi_{\parallel} + \beta \lambda n_x^2 \Pi_{\parallel}) \Delta_{\mathbf{k}}^{-1}, \\ K_{xy} = K_{yx} = -\beta \lambda \Pi_{\parallel} \Pi_{\perp} n_x n_y \Delta_{\mathbf{k}}^{-1}, \\ \Delta_{\mathbf{k}} = (1 - \beta \Pi_{\parallel} W_{\mathbf{k}}) (1 - \beta \Pi_{\perp} W_{\mathbf{k}} + \beta \lambda \Pi_{\perp}) \\ + \beta \lambda n_x^2 (\Pi_{\parallel} - \Pi_{\perp}). \quad (39)$$

The free energy is given not by (33) but by

$$\beta(F - F_0) = \beta F^{(0)} + \frac{1}{2} \sum_{\mathbf{k}} \ln(1 - \beta \Pi_{\perp} W_{\mathbf{k}}) + \frac{1}{2} \sum_{\mathbf{k}} \ln \Delta_{\mathbf{k}}. \quad (40)$$

Unlike the expressions under the logarithm sign in (33), the quantity $\Delta_{\mathbf{k}}$ vanishes at the transition point, in accord with (39) and (36), not for all $\mathbf{k} \rightarrow 0$, but only for vectors \mathbf{k} of definite direction, namely perpendicular to the x axis, in the uniaxial case and parallel to the x axis in the biaxial case. This less-singular behavior leads to smoothing of the singularities in the corrections to the thermodynamic quantities near T_c . With this, as noted

by Levanyuk,^[6] an essential difference arises between the uniaxial and biaxial transitions. In the latter case it is possible to neglect in (40) the corrections connected with $\Delta_{\mathbf{k}}$, but the second term of the right side has the same form as in (33), and the self-consistent field expansion is as before in the powers of $\alpha_{\text{cr}} \tau^{-1/2}$, where α_{cr} is defined in (35). On the other hand, in the uniaxial case only the term with $\Delta_{\mathbf{k}}$ is singular near T_c . With the aid of (39) we find that only the correlation function K_{xx} will be singular in this case in the \mathbf{k} -representation; this function for $T > T_c$ is

$$K_{xx}(\mathbf{k}) = \Pi_{\parallel} [\tau(1 - g_1) + k^2 r_0^2 V_0 / 6W_0 + \gamma n_x^2]^{-1}, \\ \gamma = \lambda / [W_0 + \lambda \Pi_{\perp} (\Pi_{\parallel} - \Pi_{\perp})^{-1}]; \\ K_{xx}(\rho) = \Pi_{\parallel} 3(4\pi r_0^2 \rho)^{-1} \\ \times \exp[-(3\gamma)^{1/2} 2^{-1/2} r_0^{-1} (\rho - |\rho_x|)], \\ r_0 \gamma^{-1/2} \ll \rho \ll r_0 \tau^{-1/2}. \quad (41)$$

Here g_1 , λ , and W_0 are the same as in (34) and (36), and the potential is taken spherically symmetrical for simplicity. Unlike the Ornstein-Zernike case (13), the decrease of the correlation with increasing distance near the transition follows a power law only for directions along the tetragonal axis.

The corrections to the thermodynamic quantities in the uniaxial case, according to (40), have the following form:

$$s^2 = \frac{3g_0^2 \tau (1 - g_1)}{g_2} \left(1 + \frac{\alpha_0}{2} \ln \frac{\gamma}{\tau} \right), \\ C_+ = C_0 + \frac{g_0 (1 - g_1)^2 \alpha_0}{g_2} \frac{1}{8} \ln \frac{\gamma}{\tau}, \\ C_- = C_0 + \frac{g_0 (1 - g_1)^2}{g_2} \left(\frac{3}{2} + \frac{\alpha_0}{2} \ln \frac{\gamma}{\tau} \right), \\ \left. \frac{\partial E_x}{4\pi \partial \mathcal{F}_x} \right|_{E=0} \Big|_{T \rightarrow T_c^+} \equiv \varepsilon_+^{-1} = \frac{\tau (1 - g_1) T_c}{\lambda g_0} \left(1 - \frac{\alpha_0}{4} \ln \frac{\gamma}{\tau} \right), \\ \varepsilon_-^{-1} = \frac{2\tau (1 - g_1) T_c}{\lambda g_0} \left(1 - \frac{\alpha_0}{4} \ln \frac{\gamma}{\tau} \right), \\ \alpha_0 = \frac{3g_2}{2\pi g_0 r_0^3} \left(\frac{6W_0^3}{\gamma V_0^3} \right)^{1/2}. \quad (42)$$

It is assumed in (42) that $\tau \ll \gamma$, the indices $+$ and $-$ correspond, as usual, to regions above and below T_c , and $C_0(T)$ denotes the regular part of the heat capacity. Comparison of (42) with (18) shows that the corrections to the zeroth approximation are of the order of $\alpha_0 \ln \tau$ in place of $\alpha \tau^{-1/2}$.

As before, we can calculate by the method of formulas (22)–(25) the next higher approximation

and verify that the order of the corresponding corrections is $(\alpha_0 \ln \tau)^2$. The n -th approximation contains thus $(\alpha_0 \ln \tau)^n$, so that on summing the perturbation-theory series we arrive at the logarithmic situation widely discussed in connection with problems in quantum field theory.^[16] Using the methods developed there, we can apparently here, too, sum all the higher order terms $(\alpha_0 \ln \tau)^n$, neglecting the terms $\alpha_0(\alpha_0 \ln \tau)^n$. This would make it possible, first, to consider quantitatively the region $|\alpha_0 \ln \tau| \lesssim 1$ and, second, permit in principle an experimental verification of the already mentioned methods of quantum field theory, including the unclear questions concerning the feasibility of some extrapolation of the results to the region $|\alpha_0 \ln \tau| > 1$.

Thus, the presence of dipole-dipole interaction in the uniaxial case leads to a different structure of the expansion in the self-consistent field parameter compared with the case of potentials with finite radius. In this connection, the considerations advanced earlier^[13] concerning the agreement between the form of the singularities for the phase transitions in crystals and in the usual Ising model may be applicable to the case of uniaxial ferroelectrics. If, however, the constant γ is small in the crystal in question, $\gamma < \alpha^2$, then the dipole-dipole interaction will be essential only in a narrow region near T_c . For example, in the region $\alpha^2 < \tau$ considered above, the valid formulas will be of the type (18) and (35).

5. ONE-DIMENSIONAL CASE

The self-consistent field method can be applied also to a study of one-dimensional systems. The zeroth approximation leads to the appearance of a phase transition regardless of the number of dimensions. For a large interaction radius r_0 , this approximation gives the correct behavior for the thermodynamic quantities far from the transition points—the corrections are of the order of $r_0^{-1}\tau^{-3/2}$. Actually there are no phase transitions in one-dimensional systems, and the singularity in the thermodynamic quantities is smeared out. For example, in the Ising model the spin averaged over the entire chain is equal to zero, and the quantity s in formulas (3)–(5) has the meaning of an average over a large but microscopic segment. The absence of transitions in one-dimensional systems is sometimes attributed to the existence of a continuous spectrum of excitations, starting from zero.^[17] It turns out that there is no transition in the Ising model, although there are no such excita-

tions in it. For interactions with the nearest neighbors this follows from the exact expression for the free energy $F = -T \ln 2 \cosh 2\beta J$. In the general case we can prove the absence of a transition, in the same manner as the impossibility of coexistence of phases in one-dimensional systems.^[18]

For small T the system breaks up into microscopic segments, in each of which the average spin has a definite direction. The limits of the segments can be regarded as dissolved impurity atoms. The free energy of the solution is expressed in terms of the concentration of the dissolved particles n by means of the formula (see^[18])

$$F = \tilde{F} + n\psi + nT(\ln n - 1), \quad (43)$$

where \tilde{F} is obtained in the same manner as in Sec. 2. For low temperatures, the entropy is small and ψ coincides with the energy of the boundary

$$\psi = \sum_{x>x'} V(x-x')(1 - \operatorname{sgn} x \cdot \operatorname{sgn} x') = V_0 r_0. \quad (44)$$

The average concentration n is obtained by minimizing (43), which yields $n = \exp(-\beta V_0 r_0)$. Thus, for large r_0 and small T , the size of the segments is exponentially large, and the addition to the free energy is exponentially small.

To calculate the correlation function, let us break up the chain into segments of length Δx smaller than n^{-1} , but larger than r_0 . Then the probability that one point of the solution will fall in this segment, and consequently that the spins will have opposite signs on the ends of the segments, is equal to $n\Delta x$. The probability W_m that at the end of the segment m the spin will be the same as at the start of the zeroth segment satisfies the recurrence relation

$$W_m = (1 - n\Delta x)W_{m-1} + n\Delta x(1 - W_{m-1}). \quad (45)$$

Solving this equation and summing over the initial and final states, we obtain for the correlation function

$$K(r) = \langle \sigma_0 \sigma_r \rangle = \exp(-r/r_c), \\ r_c = (2n)^{-1} = 1/2 \exp(\beta V_0 r_0). \quad (46)$$

This answer agrees with the exact solution for the case of nearest-neighbor interaction ($r_0 = 1$, $V_0 = 2J$):

$$K(r) = \operatorname{th}^r \beta J \approx \exp\{-2r \exp(-2\beta J)\}.$$

There are likewise no phase transitions in other one-dimensional systems. In a one-dimensional Bose gas, when calculating $K(5)$ for large r , the states of importance are those with small mo-

menta, where the occupation numbers are large, and therefore the quantum field can be replaced by a classical two-component field^[13]

$$\rho_1 = \rho \cos \varphi = 2^{-1}(a + a^+), \rho_2 = \rho \sin \varphi = i2^{-1}(a^+ - a):$$

$$K(r) = \left(\int \prod_x d^2 \rho_x \exp \left\{ -\beta \int dx \left[\frac{\hbar^2}{2m} \left(\frac{\partial \rho_x}{\partial x} \right)^2 - \mu \rho_x^2 + \frac{g}{2} \rho_x^4 \right] \right\} \right)^{-1} \int \prod_x d^2 \rho_x \rho_0 \rho_r \exp \left\{ i(\varphi_0 - \varphi_r) - \beta \int dx \left[\frac{\hbar^2}{2m} \left(\frac{\partial \rho_x}{\partial x} \right)^2 - \mu \rho_x^2 + \frac{g}{2} \rho_x^4 \right] \right\}. \quad (47)$$

Continual integrals of this kind were calculated in Feynman's paper,^[19] where the role of the coordinate x was assumed by the time t multiplied by i . Using the methods of that paper, we can obtain for K the expression

$$K(r) = \int d^2 \rho \psi_0(\rho) \rho e^{i\varphi} e^{r\hat{H}} \rho e^{-i\varphi} e^{-r\hat{H}} \psi_0(\rho) \\ = \sum_m |(\rho e^{i\varphi})_{m0}|^2 e^{-(E_m - E_0)r}, \quad (48)$$

where

$$\hat{H} = -\frac{mT}{2\hbar^2} \frac{\partial^2}{\partial \rho^2} - \mu \beta \rho^2 + \frac{\beta g}{2} \rho^4,$$

ψ_0 is the wave function of the ground state of the operator H .

At large distances, the main contribution to the sum over m in (48) is made by the first excited state with momentum 1. For small T its energy can be easily obtained by perturbation theory.

As a result we have

$$K(r) = n \exp(-r/r_c), \quad r_c = 2n\hbar^2/mT, \quad (49)$$

where $n = \langle a^+ a \rangle = \langle \rho^2 \rangle = \mu/g$ is the particle density corresponding to the chemical potential μ .

In one-dimensional superconductors, the correlation function for small T also has the form (49).^[20] Such a power-law dependence of the correlation radius on T is connected with the fact that in a Bose gas and in a superconductor the field is complex, and the Hamiltonian does not depend on its phase, so that degeneracy exists with respect to a continuous phase transformation. In the Ising model, where the degeneracy has a finite multiplicity (twofold), the correlation radius is exponentially large.

6. CONCLUSION

Thus, for a large interaction radius $r_0 \gg 1$, the self-consistent-field approximation describes well

the phase transitions in crystals and in the Ising model everywhere, except in a narrow region near the transition point. In a wide range of temperatures $T_c \gg |T - T_c| \gg T_c r^{-6}$ the thermodynamic quantities, such as the specific heat, susceptibility, spontaneous moment, all have a temperature dependence, which follows from the phenomenological theory. The correlation function in this region has the same form as the Ornstein-Zernike function. The assumption that the interaction radius is large ($r_0^3 \gg 1$) is apparently confirmed by experiment, since deviations from the phenomenological theory are observed only in a temperature region which is narrow compared with T_c . We have obtained above corrections to the zeroth approximation of the self-consistent field wherever the corrections were small.

The experimental data known to the authors do not make it possible to establish the temperature dependence of the deviations from the phenomenological theory. In those cases where the sign of these deviations has been established, it coincides with the results obtained above. The sign of the deviations is confirmed also by computer calculation of the Ising model.

We have considered above potentials in which the Fourier component $V_{\mathbf{k}}$ has a sharp positive maximum at $\mathbf{k} = 0$. In the case when the potential has a maximum $V_{\mathbf{k}_0} > 0$ at $\mathbf{k} \neq 0$, a transition of the antiferromagnetic type will take place in the system. If this maximum is not sharp, for example if the potential is a monotonic repulsion potential, then the self-consistent-field approximation is nowhere applicable. Therefore, if we assume that the potentials in ordered alloys and in antiferroelectrics are not modulated in a special manner, then phase transitions in these systems should be less adequately described by the phenomenological theory.

The phenomenological theory is best applicable to superconductors,^[3] where the role of the interaction radius is played by the pair size, which is much larger than the distance between the electrons. For the first correction to the free energy above the transition we obtain, in analogy with (14) and (33)^[12]

$$\beta F^{(1)} = 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \ln(1 - g\Pi(\mathbf{k})), \\ \Pi(\mathbf{k}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{1 - n_{\mathbf{p}} - n_{\mathbf{p}+\mathbf{k}}}{\varepsilon_{\mathbf{p}} + \varepsilon_{\mathbf{p}+\mathbf{k}}} \approx \frac{1}{g} \\ + \left[\tau + \left(\frac{kp_F}{7mT_c} \right)^2 \right] \frac{mp_F}{2\pi^2}. \quad (50)$$

The correction to the heat capacity of the form of (18):

$$C_+ = 0,3(T_c / \mu)^3 \tau^{-1/2}. \quad (51)$$

We see from this formula that the correction becomes comparable with the magnitude of the jump $0.03T_c\mu^{-1}$ only in a very narrow region $r \sim (T_c\mu^{-1})^4 \sim 10^{-16}$. A similar expansion in powers of $\tau^{-1/2}$ is obtained in a weakly nonideal Bose gas. The role of the small parameter r_0^{-3} is played in this case by the quantity $g(Tm^3)^{1/2}$. In real liquid helium, this parameter is of the order of unity and therefore there is no region where the self-consistent field approximation is applicable.

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