Perturbation theory in the phase-transition problem in the field model of a ferroelectric

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A method for calculating the correlation corrections to the results of the Landau phenomenological theory is described for the case of a displacement-type ferroelectric phase transition. First- and second-order corrections for the order parameter, the susceptibility, and the specific heat above and below T_c are found. The small parameter in powers of which the perturbation-theory series is constructed is in this case the quantity $\gamma = \sqrt{\alpha}/cq_D$, where $\sqrt{\alpha}$ corresponds to an imaginary bare "gap" in the spectrum of the critical branch and cq_D is the Debye frequency. A comparison of the derived formulas with their analogues for the Ising model [6] reveals a curious feature: The numerical coefficients of the dominant terms of the expansions (as $T-T_c \to 0$) turn out to be equal for both models, which, apparently, is a reflection of the universality of critical behavior.

1. INTRODUCTION

The problem of the computation of the correlations to the results of the Landau phenomenological theory has been considered in quite a number of papers. Following the publication of Ginzburg's well-known paper[1], the first correction was computed by Levanyuk[2,3], using as an example ferroelectric phase transitions. Subsequently, Vaks[4,5] calculated the correction in the framework of a microscopic theory. Vars, Larkin, and Pikin in[6,7] and Thouless in[8] have worked out for the Ising and Heisenberg models iterative methods that allow the determination of the corrections to the Landau theory to any order with the aid of the corresponding diagram technique.

From the point of view of the theory of ferroelectrics, the Ising model describes an order-disorder type of phase transitions. There is, however, a large number of substances that undergo displacive-type ferroelectric or structural transitions. The most important features of these transitions are reflected by a simple field model with the Hamiltonian

$$H=\int_V d\mathbf{x}\left[\frac{c^2}{2}(\nabla\varphi)^2-\frac{\alpha}{2}\varphi^2+\frac{\beta}{4!}\varphi^4\right], \tag{1}$$

where $\varphi(\mathbf{x})$ corresponds to the critical branch of the spectrum of the system, and the constants α and β are positive and small. The last restriction, which will be quantitatively defined below, is peculiar precisely to phase transitions of the displacive type. Indeed, if we allow α and β to be large, then, as is noted in[9], the Hamiltonian (1) becomes practically equivalent to the Hamiltonian of the Ising model.

In the present paper we describe a method for computing the correlation corrections in the model (1) on the basis of a diagrammatic expansion in the anharmonic-interaction constant β. This problem is, in a sense, the alternative to the situation considered in[6], where the basis of the analysis is, roughly speaking, an expansion in powers of the constant c^2 (in our notation). Accordingly, the small parameter determining the limits of applicability of the Landau theory will turn out to be quite different. It should be noted that a similar problem has been solved before in[4,5], but the use of an extremely complex model made the calculations very unwieldy even in the first approximation and above the transition point. In our case, however, the simplicity of the model (1) will allow us to find without any fundamental difficulties the first- and second-order corrections to the susceptibility, the spontaneous polarization, and the specific heat both above and below T_c, and to compare them with the analogous results for the Ising model. Let us also note the following circumstance. Several papers[10-13] have lately been published in which attempts are made to go beyond the Landau theory in problems with Hamiltonians of the type (1) with the aid of the so-called self-consistent phonon approximation. However, an incorrect interpretation of the obtained results has led in certain cases to false or questionable conclusions (for a detailed discussion and a critique, see[14]). This, in our opinion, lends an additional methodological interest to the problem of the construction of the correct iterative scheme in the case in question.

2. THE ZEROTH APPROXIMATION

Let us consider the thermodynamic Green function in the classical limit:

$$D(\mathbf{q},T)=\frac{1}{T}\int_V\langle(\varphi(\mathbf{x})-U)(\varphi(0)-U)\rangle e^{i\mathbf{q}\mathbf{x}}\,d\mathbf{x}, \tag{2}$$

where $U=\langle\varphi(\mathbf{x})\rangle$ is the order parameter. If we expand the polarization operator $\Pi(\mathbf{q},T)$ in the Dyson equation

$$D^{-1}(\mathbf{q},T)=D_0^{-1}(\mathbf{q})-\Pi(\mathbf{q},T) \tag{3}$$

in a diagram series[1)] in the bare propagators

$$D_0(\mathbf{q})=(c^2q^2-\alpha)^{-1}, \tag{4}$$

then each order of the corresponding analytic expressions will contain diverging integrals. This is, in the final analysis, connected with the instability of the system described by the unperturbed Hamiltonian. The perturbation $\beta\varphi^4$, which stabilizes the system, plays an extremely important role in the present case, and it should be taken into account in the construction of even the zeroth approximation. Bearing this in mind, let us take as the initial Green function the first-order—in the the constant β—solution $D^{(0)}(\mathbf{q},T)$ to the Dyson equation. As is easy to show[14], $D^{(0)}(\mathbf{q},T)$ has the form

$$D^{(0)}(\mathbf{q},T)=(\alpha\varkappa_0^2+c^2q^2)^{-1}, \tag{5}$$

and the inverse dimensionless correlation length κ_0 satisfies the equation

$$\varkappa_0^2=-1+t(1-\gamma\varkappa_0\operatorname{arcctg}\gamma\varkappa_0)+u^2/2. \tag{6}$$

Here

$$t=\frac{T}{T_c^{(0)}},\quad T_c^{(0)}=\frac{4\pi^2c^2\alpha}{\beta q_D},\quad u=U\sqrt{\frac{\beta}{\alpha}},\quad \gamma=\frac{\sqrt{\alpha}}{cq_D},\tag{7}$$

$q_D \sim a^{-1}$ is the cutoff momentum. The order parameter can be found from the condition of thermodynamic equilibrium, i.e., by integrating with respect to U the relation[15]

$$\partial^2F/\partial U^2=D^{-1}(0,T)\tag{8}$$

(F is the free energy) and equating the result to zero.

In the case of a phase transition of the displacive type the parameter $\gamma \ll 1$. Indeed, $\sqrt{\alpha}$ corresponds to an imaginary bare "gap" in the spectrum of the critical branch, which has an anomalously small magnitude (see, for example,[4]), while $cq_D \sim \Theta/\hbar \gg \sqrt{\alpha}$, where Θ is the Debye temperature. Furthermore, as the evaluation of the diagrams for $\Pi(q, T)$ and the vertex part and certain qualitative arguments[14] show, the dimensionless constant of the expansion in the present problem is precisely the parameter γ. Therefore, to find the dimensionless order parameter u and the dimensionless susceptibility $\chi = \alpha D(0, T)$ in the zeroth approximation, we must neglect in (6) and (8) the terms of order higher than the zeroth in γ. After the integration of (8) with respect to U, this yields

$$\varkappa_0^2=t-1+u^2/2,\tag{9}$$

$$u(t-1)+u^3/6=0.\tag{10}$$

Introducing the variable $\tau = |t - 1|$, we can write the solution to Eqs. (9) and (10) in the form

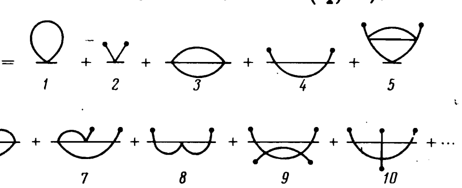
$$\chi_+^{-1}=\tau,\quad \chi_-^{-1}=2\tau,\quad u^2=6\tau,\tag{11}$$

which, obviously, coincides with the results of the Landau theory.

3. THE FIRST- AND SECOND-ORDER CORRECTIONS TO THE SUSCEPTIBILITY AND ORDER PARAMETER

To find the corrections to the phenomenological theory, let us represent $\Pi(q, T)$ in the form of a diagrammatic series in the functions $D^{(0)}(q, T)$:

$\Pi(q,T) =$



(12)

where the lines with points correspond to the order parameter U. In the expansion (12) there are no diagrams containing in the internal lines polarization inserts with one vertex, which is easy to understand, remembering the definition of $D^{(0)}(q, T)$. The susceptibility χ can be computed on the basis of the relation

$$\chi^{-1}=\varkappa_0^2-\tilde{\Pi}(0,T)\alpha^{-1},\tag{13}$$

where the polarization operator $\tilde{\Pi}$ differs from Π by the absence of the first two diagrams in (12). The order parameter will be determined with the aid of the formula (8) and the condition $\partial F/\partial U = 0$.

The distinctive feature of our problem consists in the fact that in each subsequent approximation in γ the basic Green function $D^{(0)}(q, T)$, or, more exactly, the parameter κ_0, should be redetermined. Therefore, $D^{(0)}(q, T)$ is, generally speaking, not the zeroth-order Green function; it only serves as the basis for the corresponding diagrammatic expansions. On account of this, the choice of the diagrams in each order will be made not according to the number of vertices, but according to which power of γ the contribution of the diagram in question is proportional to. In particular, in computing χ^{-1} in the first approximation, it turns out to be necessary to take the two-vertex diagram 4 in (12) into account. This, however, does not mean that there is no connection at all between the number of vertices of a diagram and the power of γ. As is easy to show, the increase of the number of vertices of a diagram leads to the monotonic increase of the power of γ, to which the corresponding contribution is proportional; in this sense the expansion (12) is quite adequate for the formulated problem.

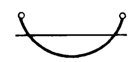
So, let us express κ_0^2 in terms of u^2 up to the first order in γ. Solving the equation

$$\varkappa_0^2=t-1-\frac{\gamma\pi t}{2}\varkappa_0+\frac{u^2}{2},\tag{14}$$

which is obtainable from (6) by expanding the arc tangent, we have

$$\varkappa_0^2=\frac{u^2}{2}+t-1-\frac{\gamma\pi t}{2}\left(\frac{u^2}{2}+t-1\right)^{1/2}.\tag{15}$$

The diagram 4 in (12) also gives a contribution of the order of γ to χ^{-1}:



$$=\frac{T\beta^2U^2}{2(2\pi)^3}\int\frac{dq}{(\alpha\varkappa_0^2+c^2q^2)^2}\approx\frac{\alpha\gamma\pi tu^2}{4\varkappa_0}.\tag{16}$$

Since $\chi^{-1} = D^{-1}(0, T)/\alpha$, the equation for the determination of u can be obtained by substituting into (13) the expression (16) for $\Pi(0, T)$ in the first approximation and then integrating (13) with respect to u with allowance for (15). This equation has the form

$$\frac{u^3}{6}+u(t-1)-\frac{\gamma\pi t}{2}u\left(\frac{u^2}{2}+t-1\right)^{1/2}=0.\tag{17}$$

Iterating (17) up to first oder in γ, we find u^2 in the first approximation:

$$u^2=6\tau(1+\sigma\sqrt{2/\tau}).\tag{18}$$

Here we have introduced the parameter $\sigma = \gamma\pi/2$, and have also dropped in the brackets the term that vanishes as $\tau \to 0$. Further, we can find the inverse susceptibility χ^{-1}. Combining (13), (15), (16), and (18), and again neglecting the nonsingular—in the temperature—term, we obtain

$$\chi_-^{-1}=2\tau(1+\sigma/\sqrt{8\tau}).\tag{19}$$

The computation of χ^{-1} above the Curie point is elementary. From (13) and (15) we at once find

$$\chi_+^{-1}=\tau(1-\sigma/\sqrt{\tau})\tag{20}$$

As was to be expected, the correction terms in (18)—(20) are similar in form to the corrections found earlier in[2,4-6]. Of considerably greater interest, however, is the fact that the results obtained above for the field model also coincide quantitatively (i.e., right up to the numerical coefficients) with the corresponding formulas for the Ising model[6] 2), the only difference being that the formulas (18)—(20) and the analogous formulas obtained in[6] contain different small parameters (σ and $\alpha = 3\sqrt{6}/2\pi r_0^3$, where r_0 is the interaction radius) that are of different physical nature and that cannot be transformed into each other with the aid of a transformation of the model constants. The question arises whether the coincidence of the numerical coefficients of the first-order corrections for the model (1) and the Ising model is not fortuitous. This question can be answered (with a definite degree of certainty) after computing the second-order corrections to χ^{-1} and u^2 for the field model and comparing them with the results obtained by Vaks, Larkin, and Pikin. With the same end in view, we shall also find the first- and second-order corrections to the specific heat.

The diagrams that must be taken into account when determining χ^{-1} and u^2 in the second approximation are given in (12). The diagram 3 has already been computed in[14]; the corresponding analytic expression has, up to terms that are unimportant for $\tau \to 0$, the form

$$-{}^1/_3\alpha\sigma^2 \ln b\gamma^2\varkappa_0^2, \quad b\approx 19. \tag{21}$$

The external momentum here has been assumed, in accordance with (13), to be equal to zero. On account of this same condition, the diagram 5 in (12) differs from the diagrams 6 and 7 only in having a different combinatorial factor; their combined contribution is equal to

$$-\frac{5}{4}\frac{T^2\beta^2U^2}{(2\pi)^6}\int dq\,dq' D^{(0)2}(q)D^{(0)}(q')D^{(0)}(q+q') \approx -\frac{5\alpha\sigma^2u^2}{6\varkappa_0^2}. \tag{22}$$

It is convenient to evaluate the integral in (22) not directly, but through the differentiation with respect to $\alpha\kappa_0^2$ of the diagram integral (21) with allowance for the fact that an invariant-cutoff condition on the momentum q_D is implied in both integrals. Differentiating in its turn the integral (22), we can also find the sum of the last two diagrams in (12). It is equal to

$$\approx \alpha\sigma^2u^4/6\varkappa_0^4. \tag{23}$$

Finally, the evaluation of the diagram 8 in (12) yields

$$\approx -\alpha\sigma^2u^2/4\varkappa_0^2. \tag{24}$$

In the last three expressions, we have, as in (21), retained only the terms that are dominant for $\tau \to 0$.

The course of the subsequent computations remains the same as in the calculation of the first-order corrections. The equation for the order parameter has the form

$$\frac{u^3}{6} - \tau u - \sigma u\sqrt{\frac{u^2}{2}-\tau} + \tau + \sigma^2\left\{\frac{u}{3}\ln\left[b\gamma^2\left(\frac{u^2}{2}-\tau\right)\right] + \frac{\tau u}{3(u^2/2-\tau)} + \frac{5}{6}u\right\} = 0. \tag{25}$$

Solving it iteratively, we obtain

$$u^2 = 6\tau\left(1+\sigma\sqrt{\frac{2}{\tau}} + \frac{\sigma^2}{2\tau} - \frac{\sigma^2}{3\tau}\ln 2\tau b\gamma^2\right). \tag{26}$$

Further, we can find the susceptibility in the ordered phase:

$$\chi_-^{-1} = 2\tau\left(1+\frac{\sigma}{\sqrt{8\tau}} + \frac{3\sigma^2}{8\tau} - \frac{\sigma^2}{3\tau}\ln 2\tau b\gamma^2\right). \tag{27}$$

The computation of the susceptibility above the Curie point presents no difficulty; the result has the form

$$\chi_+^{-1} = \tau\left(1-\frac{\sigma}{\sqrt{\tau}} + \frac{\sigma^2}{2\tau} + \frac{\sigma^2}{3\tau}\ln \tau b\gamma^2\right). \tag{28}$$

We defer the discussion of the formulas (26)—(28) to the final section, and proceed now to the computation of the singular part of the specific heat.

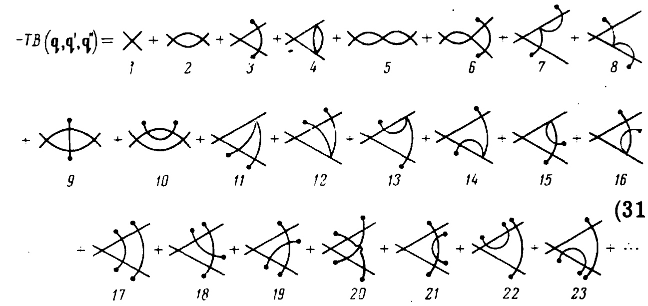
4. THE SPECIFIC HEAT IN SECOND-ORDER PERTURBATION THEORY

It is convenient in our case to compute the specific heat with the aid of the relation[15]

$$C = -\frac{\beta C_0}{2}\left[\frac{\partial^2 F}{\partial\alpha^2} - \left(\frac{\partial^2 F}{\partial\alpha\,\partial U}\right)^2 \Big/ \frac{\partial^2 F}{\partial U^2}\right], \quad C_0 = \frac{2T_c}{\beta}\left(\frac{d\alpha}{dT_c}\right)^2, \tag{29}$$

it being necessary in the determination of the specific heat above the phase-transition point to drop the second term in the square brackets. The derivatives of the free energy entering into (29) can be represented in the form of a sum of vertex diagrams of a definite type[15]. Thus, $\partial^2F/\partial\alpha\partial U$ is expressible as a sum of diagrams with one angle:

$$\frac{\partial^2 F}{\partial\alpha\,\partial U} = -\frac{1}{\beta}\int B(0,0,0)\,dU, \tag{30}$$



(31)

which can be easily verified by substituting (8) into the Ward identity

$$\partial D^{-1}(0, T)/\partial\alpha = -B(0, 0, 0)/\beta. \tag{32}$$

The derivative $\partial^2F/\partial\alpha^2$ is equal up to a constant factor to the sum of the diagrams with two angles:

$$\partial^2 F/\partial\alpha^2 = \tilde{B}(0, 0, 0)/\beta^2, \tag{33}$$

where $T\tilde{B}(q, q', q'')$ includes the diagrams 2, 5, 9, and 10 from the diagrams shown in (31). The computation of the specific heat thus reduces to the evaluation of the diagrams for $B(0, 0, 0)$ and $\tilde{B}(0, 0, 0)$, the integration of $B(0, 0, 0)$ over U, and the substitution into the obtained formulas of the previously-found expression for u.

It is not difficult to show that the evaluation of the first diagram (the bare vertex) yields the results of the phenomenological theory; the jump in the specific heat turns out in this case to be equal to $^3/_2C_0$. Allowance for the next two diagrams allows us to obtain the first-order corrections to the Landau theory. Finally, to find the specific heat in the second approximation, we must take all the remaining diagrams in (31) into account. The principle by which the diagrams in (31) are chosen becomes clear if we notice that the power of γ, to which the contribution of the diagram for B or $\tilde{B}$ is proportional, is connected with the number m of vertices and the number l of lines with points by the relation

$$n = m - l/2 - 1. \tag{34}$$

Let us briefly discuss the evaluation of the diagrams on the second and third lines in (31). Each of them can, generally speaking, be found, say, with the aid of the Feynman parametrization method. It is more convenient, however, to evaluate at once the sums of the diagrams on each line, noting that they are expressible in terms of (23). In fact, because the external momenta are equal to zero, the diagrams 13—16 on the second line are equal to the diagram 10, while the diagrams 11 and 12 differ from the diagram 9 only in having different numerical coefficients, the combinatorial factors of these eight diagrams being such that their sum is simply proportional to (23). In its turn, the contribution of the seven diagrams of the third line can be obtained from (23) by differentiating the corresponding integrals with respect to $\alpha\kappa_0^2$. Finally, the sum of all the fifteen diagrams 9—23 is equal to

$$\approx 5\sigma^2 u^2/6\varkappa_0^4 - \sigma^2 u^4/3\varkappa_0^6. \tag{35}$$

The computation of the remaining diagrams for B(0, 0, 0) is elementary. Integrating then B(0, 0, 0) over U with allowance for (15), and substituting (26) into the resulting expression, we obtain

$$C_- = C_0(3/2 + \sigma/\sqrt{2\tau} - \sigma^2/2\tau). \tag{36}$$

The calculation of the specific heat in the disordered phase yields

$$C_+ = C_0\sigma/4\sqrt{\tau} + O(\sigma^3). \tag{37}$$

Notice that the second-order correction to the specific heat above the Curie point is identically equal to zero.

5. DISCUSSION OF THE RESULTS

So, we have found the first two correction terms for the susceptibility, order parameter, and specific heat in the case of a displacive-type phase transition. As has already been noted, it is of interest to compare our results with the analogous formulas for the Ising model[6]:

$$\begin{gathered} u^2 = 3\tau\left(1+\alpha\sqrt{\frac{2}{\tau}}+\frac{\alpha^2}{2\tau}-\frac{\alpha^2}{3\tau}\ln 32\tau\right),\\ \chi_-^{-1} = 2T_c\tau\left(1+\frac{\alpha}{\sqrt{8\tau}}+\frac{3\alpha^2}{8\tau}-\frac{\alpha^2}{3\tau}\ln 32\tau\right)\\ \chi_+^{-1} = T_c\tau\left(1-\frac{\alpha}{\sqrt{\tau}}+\frac{\alpha^2}{2\tau}+\frac{\alpha^2}{3\tau}\ln 16\tau\right),\\ C_- = \frac{3}{2}+\frac{\alpha}{\sqrt{2\tau}}-\frac{\alpha^2}{2\tau}, \quad C_+ = \frac{\alpha}{4\sqrt{\tau}}+\frac{\alpha^3}{12\tau^{3/2}}\left[\ln\frac{1}{\tau}-2\ln\frac{16}{3}+2\right]. \end{gathered} \tag{38}$$

It is quite evident that in the first approximation the results for the field model and the Ising model coincide up to the replacement of σ by the small Vaks-Larkin-Pikin parameter α. Let us recall, however, that above we neglected everywhere the terms that were small for $\tau \to 0$, and therefore the last assertion is valid only for $\tau \ll 1$. In the second order the corrections to u and χ^{-1}, besides terms of the type σ^2/τ, also contain a logarithmic term, the numerical coefficients in front of $\tau^{-1}\ln\tau$ for both models being equal and those in front of τ^{-1} being different[3)]. Since the region of applicability of the perturbation theory is limited by the condition $\tau \gg \gamma^2$, the second-order corrections to u and χ^{-1} in the Ising and field models are significantly different. However, the equality of the coefficients in front of $\tau^{-1}\ln\tau$, as well as the equality of the coefficients of the second-order corrections to the specific heat, is, apparently, not accidental. The point is that as we approach the critical region the logarithmic term becomes dominant, and the coincidence of the coefficients of the dominant terms of the expansions for the different models probably reflects the universality of critical behavior. This fact is also in accord with the possibility, first noted by Gor'kov and Pitaevskiĭ[16], of reducing the statistical sum for the phonon gas to the statistical sum of the Ising model in the strong-coupling case.

In conclusion, I should like to thank V. G. Vaks and N. M. Plakida for a discussion of the results of the paper and A. A. Abrikosov for his comments.

1)The technique employed here is described in greater detail in [14,15].

2)Nontrivial here is, of course, the coincidence of the coefficients for the two models in only two of the three formulas (say, in the expressions for χ_+^{-1} and χ_-^{-1}), since the parameter σ was introduced precisely on the basis of a comparison of the third formula (for u^2) with the analogous relation for the Ising model.

3)The coefficients in front of α^2/τ contain $ln\,32$ or $ln\,16$, whereas those in front of σ^2/τ contain $\ln 2b\gamma^2$ or $\ln b\gamma^2$.

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