Self-Consistent Treatment

of a Phase Transition

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A self-consistent treatment of a phase transition with a scalar order parameter in the ordered and disordered state is described. The factorization of the correlation functions in the disordered phase leads to a shift of the transition temperature, a linear divergence ($\nu = 1$) for the correlation length, a quadratic divergence ($\gamma = 2$) for the susceptibility, and a finite value ($\alpha = -1$) for the specific heat. In the ordered phase the factorization of the correlation functions leads to no divergences in the correlation length and susceptibility. A study of the free energy shows that order persists above the transition temperature found by assuming disorder. The requirement of thermodynamic stability induces a first-order transition at a temperature which lies between the bare transition temperature and the shifted one.

1. INTRODUCTION

In a previous paper[1] (hereafter referred to as I) we presented a formalism based on field-theory techniques for the description of continuous phase transitions.

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The partition function was written as a functional integral

$$Z = \int \mathscr{D}\{\eta\} \exp[-\beta F\{\eta(\mathbf{x})\}] \tag{1}$$

where $\eta(\mathbf{x})$ is a local, scalar order parameter defined on a coarse-grained space and β is the inverse temperature $(k_B T)^{-1}$. The functional $\exp[-\beta F\{\eta(\mathbf{x})\}]$ gives the statistical weight of a prescribed order parameter configuration after all other variables have been summed over.

The model is defined by the form of the functional $F\{\eta\}$. For the sake of generality in I we considered

$$F\{\eta\} = A(12)\,\eta(1)\,\eta(2) + B(1234)\,\eta(1)\,\eta(2)\,\eta(3)\,\eta(4) - \mu(1)\,\eta(1) \tag{2}$$

with $1 = \mathbf{x}_1$, $2 = \mathbf{x}_2$, etc., and volume integration over repeated indices. In the present calculation we will use the Landau–Ginzburg[2] form for A and B, namely

$$A(12) = (A - A_0\nabla^2)\,\delta(1 - 2), \qquad B(1234) = B\delta(1 - 2)\,\delta(2 - 3)\,\delta(3 - 4) \tag{3}$$

with

$$A = \alpha(T - T_c), \qquad \alpha > 0, \quad B > 0, \quad T_c > 0$$

T_c is the bare transition temperature.

The n-point order parameter correlation function is obtained taking the ensemble average of the product of n field variables

$$\langle \eta(1)\,\eta(2) \cdots \eta(n)\rangle = Z^{-1} \int \mathscr{D}\{\eta\}\,\eta(1)\,\eta(2) \cdots \eta(n)\,e^{-\beta F\{\eta\}} \tag{4}$$

Most physical quantities of interest in the critical region can be expressed in terms of the average order parameter

$$g(1) = \langle \eta(1)\rangle \tag{5}$$

and the two-point cumulant

$$q(12) = \langle [\eta(1) - g(1)][\eta(2) - g(2)]\rangle \tag{6}$$

The equations satisfied by g and q were derived in I. These equations are formally analogous to the equations of motion for the condensate and the two-point Green's function in quantum many-body theory.[3]

In particular, the equation for $q(12)$ takes the form of Dyson's equation

$$q^{-1}(12) = q_0^{-1}(12) - M(12) \tag{7}$$

where

$$q_0^{-1}(12) = 2\beta A(12) \tag{8}$$

and $M(12)$, the analog of the self-energy, is a functional of g and q. In the disordered phase, where the average order parameter is zero, Eq. (7) is the only equation to be considered.

Expanding M in skeleton diagrams[4] gives self-consistent approximation schemes.

The most simple approximation of this type is the Hartree approximation, where only the first-order contribution to M is retained. In Fourier space this leads to a self-energy independent of $\mathbf{k}$. A feature of this approximation is that all higher correlation functions factorize in terms of the two-point correlation function. Consequently, the Hartree approximation cannot be expected to hold in the immediate neighborhood of the transition, where the large, long-wavelength fluctuations are strongly interacting.

From a different poin of view, the Hartree approximation emerges on replacing the Landau–Ginzburg free energy functional

$$F = \int d^3x \, [A_0(\nabla\eta)^2 + A\eta^2(\mathbf{x}) + B\eta^4(\mathbf{x})] \tag{9}$$

by the linearized form

$$\int d^3x \, \{A_0(\nabla\eta)^2 + [A + 6B\langle\eta^2(\mathbf{x})\rangle] \, \eta^2(\mathbf{x}) - 3B\langle\eta^2\rangle^2\} \tag{10}$$

in the exponential of equation (1). The factors 6 and 3 are combinatorial factors appropriate to a scalar classical field. Finally, $\langle\eta^2(\mathbf{x})\rangle$ is to be determined self-consistently from Eq. (4).

The factorization of the correlation functions then follows from the Gaussian character of the statistical weight.

The interest of this approximation is that it gives a first, nontrivial correction to the classical theory.

Here we follow the approximation to its logical conclusions. It is a self-consistent theory and does not break down on its own accord. However, the consideration of further terms in the exact theory sets limits to the region in which the present approximation can be a good approximation. These limits are discussed in Section 7. Murata and Doniach's[17] treatment of the weak itinerant ferromagnet, which came to our attention after the completion of this work, has to be viewed as the same approximation as the one treated here for values of the temperature where neither the nonlinearities reported here nor those of the exact critical behavior are important.

The main results are a quadratic divergence for the susceptibility and a

linear divergence for the correlation length. In I it was shown that the cancellation of the classical terms cannot be obtained in any finite order of perturbation expansion in B for the correlation function.

In the ordered phase there is a nonvanishing average order parameter g. The equation satisfied by g was shown in I to be

$$\beta^{-1} q_0^{-1}(12)\, g(2) = \mu(1) + K(1) \tag{11}$$

where $K(1)$, the effective external field, is a functional of g and q. In order to specify an approximation in the ordered phase, both M and K have to be given. The relationships between M and K and their reflection in approximate treatments were discussed in I.

In the following we shall see that a first-order approximation for K and M fits in the scheme of the Φ-derivable approximations.[6] However, it also turns out that a first-order self-energy is insufficient to describe a continuous transition when approaching the transition from the ordered phase. A study of the free energy shows that a first-order approximation for the self-energy on both sides of the transition is consistent only with a first-order transition. The appearance of such spurious first-order transitions has been discussed by Pytte[7a] and Gillis and Koehler[7b] with regard to the self-consistent phonon approximation for displacive phase transitions.

This problem arose also in the context of Belyaev's[16] treatment of the Bose liquid. There the attainment of a gapless approximation is related to the absence of a gap in the excitation spectrum. The requirement of gaplessness leads to a very complicated integral equation which is solved by Belyaev[16] to second order in the interaction. (Compare also Ref. 6, Section 6.)

As far as the continuity of thermodynamic quantities across the transition is concerned, the condition of gaplessness [Eq. (59) below] needs to be satisfied only with respect to the zero-momentum component of the order parameter.[4] This condition can be imposed and solved exactly. It results in the spherical model. A more detailed discussion of this point will be presented elsewhere.[5]

2. OUTLINE OF THE APPROXIMATION SCHEME

The thermodynamic free energy W is related to the partition function by

$$W = -\beta^{-1} \log Z \tag{12}$$

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[4] See also concluding remarks of Section 7.
[5] One of us (D.J.A.) is indebted to Dr. Cyrano De Dominicis for a conversation in which this point was clarified.

In I we derived a Luttinger–Ward[8] expression for the free energy which is a functional of g and q and which up to a constant independent of β, A, B, and μ coincides with W:

$$W\{g, q\} = -\mu(1)\, g(1) + A(12)[\,g(1)\, g(2) + q(12)\,]$$
$$- \tfrac{1}{2}\beta^{-1} \log q(11) - \tfrac{1}{2}\Phi\{g, q\} \tag{13}$$

The notation $\log q(11)$ stands for the trace of the matrix $\log q(12)$. The functional $\Phi\{g, q\}$ is related to the quantities K and M in Eqs. (11) and (7) by

$$\left.\frac{\delta\Phi}{\delta g(1)}\right|_{q} = 2K(1), \qquad \left.\frac{\delta\Phi}{\delta q(12)}\right|_{g} = \beta^{-1}M(12) \tag{14}$$

The above expression for the free energy has the property that it is stationary for variations of g and q about their physical values when the parameters are kept fixed. The proof of the variational property requires only that g and q satisfy Eqs. (11) and (7) and that M and K are related to Φ by Eq. (14). Therefore consistent approximations for g and q can be derived by approximating the functional Φ, constructing K and M according to Eq. (14), and solving the resulting equations (11) and (7).

In this paper we shall consider the first-order contribution to Φ. Namely representing pictorially the interaction by a dot, the order parameter g by a wavy line, and the correlation function q by a straight line[1]

or analytically

$$\Phi\{g, q\} = -2B(1234)[\,g(1)\, g(2)\, g(3)\, g(4)$$
$$+ 6g(1)\, g(2)\, q(34) + 3q(12)\, q(34)\,] \tag{15}$$

Consequently, according to Eq. (14),

$$= -4B(1234)[\,g(2)\, g(3)\, g(4) + 3g(2)\, q(34)\,] \tag{16}$$

and

$$M(12) = \quad\quad + \quad\quad$$

$$= -12\beta B(1234)[g(3)\, g(4) + q(34)] \tag{17}$$

Inserting these expressions for K and M in Eqs. (7) and (11) with the form (3) for the couplings, one obtains a system of equations for g and q. In the presence of a uniform external field the system is translationally invariant and the equations for g and q take the form

$$2[A + 2B(g^2 + 3\mathcal{N})]\, g = \mu \tag{18}$$

$$2\beta[A - A_0\nabla^2 + 6B(g^2 + \mathcal{N})]\, q(\mathbf{r}) = \delta(\mathbf{r}) \tag{19}$$

where $\mathbf{r} = (1 - 2)$. $\mathcal{N}$ is to be determined self-consistently by

$$\mathcal{N} = q(11) = \lim_{2\to 1} q(12) \tag{20}$$

These equations apply both below and above the transition. Once these equations have been solved the free energy is given unambiguously by Eq. (13).

3. THE DISORDERED PHASE

In the disordered phase, namely for temperatures greater than the transition temperature and in the absence of an external field, one usually takes $g = 0$. Consequently, the $\mathbf{k}$-Fourier component of $q(\mathbf{r})$ satisfies the equation

$$q(\mathbf{k}) = [2\beta(A_0 k^2 + A + 6B\mathcal{N})]^{-1} \tag{21}$$

with

$$\mathcal{N} = (1/\Omega) \sum_{\mathbf{k}} q(\mathbf{k}) \tag{22}$$

where Ω is the volume of the system.

Transforming the sum into an integral, the requirement of self-consistency leads to the following equation:

$$\mathcal{N} = \frac{1}{4\pi^2 \beta A_0} \int_0^{\bar{p}} dk\, \frac{k^2}{k^2 + \xi^{-2}} \tag{23}$$

where the correlation length ξ is given by

$$\xi = \left(\frac{A + 6B\mathcal{N}}{A_0} \right)^{-1/2} \tag{24}$$

The momentum cutoff $\bar{p}$ has its origin in the coarse-grained nature of the field $\eta(\mathbf{x})$. As was discussed in I, the phenomenological free energy functional (2) can be thought of as the effective Hamiltonian of the system after all fluctuations with wavelength shorter than the size of the coarse-graining cells have been summed over. The size of the cells is roughly the range of the interaction $(\bar{p})^{-1}$. All components of the field with $k > \bar{p}$ are assumed to have been integrated out; consequently, the field $\eta(\mathbf{x})$ does not contain wavelengths shorter than $(\bar{p})^{-1}$.

Carrying out the integration, one obtains the following equation for the correlation length:

$$\xi^{-2} = \xi_0^{-2} + \left(\frac{T}{T_c} \right) \frac{\bar{p}}{R} - \left(\frac{T}{T_c} \right) \frac{\xi^{-1}}{R} \tan^{-1} \left(\frac{\bar{p}}{\xi^{-1}} \right) \tag{25}$$

where

$$\xi_0 = (A_0/A)^{1/2} \tag{26}$$

is the classical correlation length.[9] The quantity

$$R = 2\pi^2 A_0{}^2 / 3 B k_B T_c \tag{27}$$

is a fundamental length that separates the classical region from the non-classical region. Namely, the criterion for the validity of the classical theory takes the form $(\xi_0/R) \ll 1$.[10]

4. THE TRANSITION TEMPERATURE

The static susceptibility is related to the order parameter correlation function via[1]

$$\chi = \beta q(\mathbf{k} = 0)$$

At the transition we expect the susceptibility to diverge. Therefore we define the transition temperature T_r by

$$q^{-1}(\mathbf{k} = 0, T_r) = 0 \tag{28}$$

From Eq. (21) it follows that the above condition is equivalent to $(A_r + 6B\mathcal{N}_r) = 0$, or $\xi^{-1}(T_r) = 0$.

At temperature T

$$q^{-1}(\mathbf{k} = 0, T) = 2\beta A(\mathbf{k} = 0, T) - M(\mathbf{k} = 0, T)$$

where the self-energy M is the correction to the classical behavior.

At T_r Eq. (28) implies

$$2\beta_r A(T_r) - M(0, T_r) = 0$$

We may therefore rewrite $q^{-1}(0, T)$ as

$$q^{-1}(0, T) = 2\beta[A(0, T) - A(0, T_r)] + 2(\beta - \beta_r) A(0, T_r) - [M(0, T) \\ - M(0, T_r)]$$

If A is temperature independent, the first term on the right hand side vanishes. If it has the form (3), it is linear in $(T - T_r)$. Similarly $(\beta - \beta_r)$ is linear to lowest order. Thus the first two terms on the rhs give the classical contribution, $\gamma = 1$.

Beyond the classical theory one expects $\chi \propto (T - T_r)^{-\gamma}$ with $\gamma > 1$; in that case $[M(\mathbf{k} = 0, T) - M(\mathbf{k} = 0, T_r)]$ must contain a linear term in $(T - T_r)$ which exactly cancels the classical contribution. Furthermore, as was observed in I, a result of this type cannot be obtained in any approximation of finite order in perturbation theory.

We shall now see that in the Hartree approximation, where $M(\mathbf{k}) = -12\beta B\mathcal{N}$, the cancellation of the classical term indeed occurs.

From Eq. (25) we notice that the solution $\xi^{-1} = 0$ can occur only if $[\xi_0^{-2} + (T/T_c) \bar{p}/R] = 0$. The renormalized transition temperature is then given by

$$T_r = \frac{T_c}{1 + (r/R)} \tag{29}$$

where we have introduced the effective interaction range[10]

$$r = (A_0/\alpha T_c)^{1/2} \tag{30}$$

which is related to the momentum cutoff by $\bar{p} = r^{-1}$. For small values of ξ^{-1} Eq. (25) can be rewritten as

$$\xi^{-2} = r^{-2}\epsilon - (\epsilon + 1) \frac{T_r}{T_c} \frac{\pi}{2R} \xi^{-1} \tag{31}$$

where $\epsilon = (T - T_r)/T_r$ is the reduced temperature.

Expanding to lowest order in ϵ

$$\xi^{-1} = \frac{2}{\pi} \left(\frac{T_c}{T_r}\right) Rr^{-2}\epsilon \tag{32}$$

This result gives for the critical exponent of the correlation length $\nu = 1$.[6] The value $\gamma = 2$ for the critical exponent of the susceptibility follows immediately from the relation

$$\chi = \beta q(\mathbf{k} = 0) = \xi^2/2A_0 \tag{33}$$

This proves that the self-energy correction contains a term linear in ϵ which exactly cancels the classical contribution. From Eqs. (24) and (32), in fact, one has

$$\mathcal{N} - \mathcal{N}_r = \frac{A_0}{6B} \left[\frac{2}{\pi} \left(\frac{T_c}{T_r}\right) Rr^{-2}\right]^2 \epsilon^2 - \frac{\alpha T_r}{6B}\epsilon \tag{34}$$

In terms of the self-energy $M = -12\beta B\mathcal{N}$ the last expression means that for $\epsilon \to 0$ there is a term in M of the form $-2\beta T_r\epsilon$, which is independent of B.

In the opposite limit, namely away from the transition, one expects to recover the classical result.

In fact from Eq. (25) in the limit $\xi^{-1}/\bar{p} \to \infty$ to lowest order, one has $\xi^{-2} = \xi_0^{-2}$, which implies $\mathcal{N} = 0$. This can be clearly seen in Fig. 1, where the solution of Eq. (25) for $r/R = 0.1$ is compared to ξ_0^{-2}.

[6] For a definition of the critical exponents see Fisher.[11]
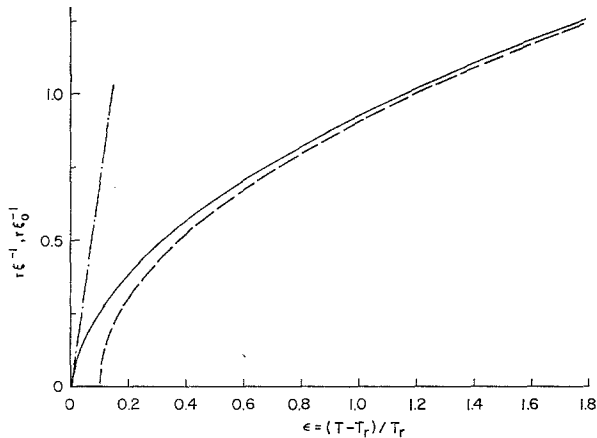

Fig. 1. Comparison of $r\xi^{-1}$ (continuous line) above the transition with its classical counterpart $r\xi_0^{-1}$ (dashed line) for $r/R = 0.1$. The dot-dash line represents the asymptotic behavior of $r\xi^{-1}$.

5. THE SPECIFIC HEAT

To complete the analysis of the disordered phase, we shall now compute the specific heat. With the form (3) for the couplings and the approximation (15) for the functional Φ, the free energy (13) becomes

$$W\{g, q(\mathbf{k})\} = \Omega(-\mu g + Ag^2 + Bg^4) + \sum_{\mathbf{k}} (A + A_0 k^2) q(\mathbf{k})$$

$$+ 6Bg^2 \sum_{\mathbf{k}} q(\mathbf{k}) + \frac{3B}{\Omega} \sum_{\mathbf{k}\mathbf{k}'} q(\mathbf{k}) q(\mathbf{k}')$$

$$- \tfrac{1}{2}\beta^{-1} \sum_{\mathbf{k}} \log q(\mathbf{k}) \tag{35}$$

In the disordered phase ($\mu = 0, g = 0$) and at equilibrium, that is, for values of $q(\mathbf{k})$ that satisfy Eq. (21), the above expression for the free energy becomes (Appendix A)

$$W\{q(\mathbf{k})\} = \sum_{\mathbf{k}} \tfrac{1}{2}\beta^{-1} - 3B\Omega\mathcal{N}^2 - \tfrac{1}{2}\beta^{-1} \sum_{\mathbf{k}} \log q(\mathbf{k}) \tag{36}$$

A similar expression for the free energy has been successfully applied by other authors[12,13] to the computation of the specific heat of a two-dimensional superconductor.[14]
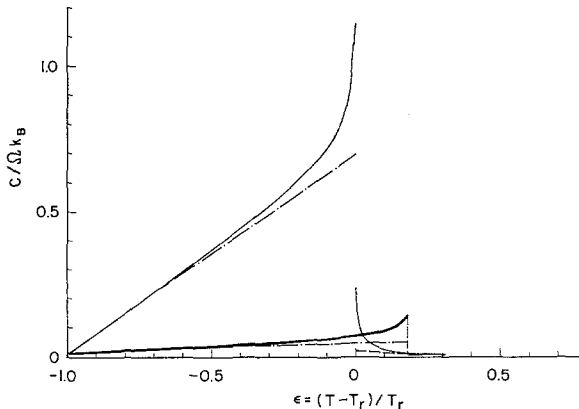

Fig. 2. Specific heat for $r/R = 0.1$ (thin continuous lines) and for $r/R = 1$ (thick continuous lines). The dot-dashed lines represent the classical specific heat for the same values of r/R. The dashed line represents the continuation of the specific heat in the region of thermodynamic instability.

The entropy and the specific heat are then given by (Appendix A)

$$S = -\Omega \frac{\partial A}{\partial T} \mathcal{N} + \frac{k_B}{2} \sum_{\mathbf{k}} \log q(\mathbf{k}) \tag{37}$$

$$C = \sum \frac{k_B}{2} - \Omega \alpha \mathcal{N} - \Omega(A + 6B\mathcal{N}) \frac{\partial \mathcal{N}}{\partial T} - \Omega \alpha T_c \frac{\partial \mathcal{N}}{\partial T} \tag{38}$$

Approaching the transition the specific heat tends linearly to a finite value (Fig. 2). In fact, for $\epsilon \ll 1$

$$C = \frac{\Omega \, \Delta C}{3} \left\{ \frac{1}{3a} + \left(\frac{a}{1+a} \right) + \left[\left(\frac{a}{1+a} \right) - \frac{8}{\pi^2} \frac{(a+1)^3}{a} \right] \epsilon \right.$$
$$\left. - 2 \left(\frac{2}{\pi} \right)^4 \frac{(a+1)^5}{a} \, \epsilon^3 \right\} \tag{39}$$

where $a = R/r$, and

$$\Delta C = \frac{\alpha^2 T_c}{2B} = \frac{3k_B a r^{-3}}{4\pi^2} \tag{40}$$

is the classical specific heat jump.

Taking the limit $B \to 0$ in the formula (38) and then letting $T \to T_c$, one obtains (see Appendix B) an asymptotic expression for the specific heat which diverges like $[(T - T_c)/T_c]^{-1/2}$.[10,15]

6. THE ORDERED PHASE

In the ordered phase the average order parameter has a nonvanishing value even in absence of an external field. Thus the physical solution of Eq. (18) for $\mu = 0$ is

$$g^2 = -(A + 6B\mathcal{N})/2B \tag{41}$$

The equation for the correlation function becomes

$$q^{-1}(\mathbf{k}) = 2\beta A_0 [k^2 + \xi^{-2}] \tag{42}$$

where the correlation length in the ordered phase is given by

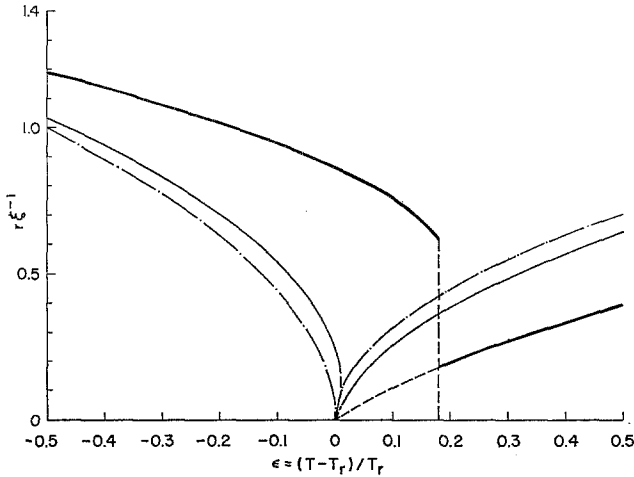$$\xi = [-2(A + 6B\mathcal{N})/A_0]^{-1/2} \tag{43}$$

Fig. 3. Self-consistent solution of Eqs. (25) and (44) for $r/R = 0.1$ (thin continuous lines) and for $r/R = 1$ (thick continuous lines). The dot-dashed lines represent the classical limit, namely $r\xi_0^{-1} = \epsilon^{1/2}$ above the transition and $r\xi_0^{-1} = (-2\epsilon)^{1/2}$ below the transition. The dashed line indicates the continuation of ξ^{-1} in a region of thermodynamic instability.

Proceeding as in Section 3, the following self-consistency relation is obtained:

$$\xi^{-2} = -2r^{-2}\epsilon + 2(\epsilon + 1)\frac{a}{a+1}\frac{\xi^{-1}}{R}\tan^{-1}\left(\frac{\bar{p}}{\xi^{-1}}\right) \qquad (44)$$

The solution of Eq. (44) is plotted in Fig. 3 for the values 1 and 0.1 of the parameter r/R. One can see that $\lim_{\epsilon \to 0^-}\xi^{-1} \neq 0$.

Thus, as T_r, the transition temperature defined assuming disorder, is approached from below the correlation length does not diverge. Similarly the susceptibility, related to ξ by Eq. (33), does not diverge and the order parameter $g^2 = (A_0/4B)\xi^{-2}$, does not vanish. However, at $\epsilon = 0$ Eq. (44) also admits the solution $\xi^{-1} = 0$. In order to clarify the origin of this additional solution and the nature of the transition, we shall now investigate the behavior of the free energy. The expression for the free energy given in Eq. (35) defines a hypersurface in the space of the infinitely many variables $\{g, q(\mathbf{k})\}$. The minima of this hypersurface correspond to the equilibrium states of the system. We want to determine how the free energy depends on g.

If $q(\mathbf{k})$ is taken at its stationary value, given by Eq. (42), and $\mathcal{N}(g)$ is the solution of

$$\mathcal{N}(g) = (1/\Omega)\sum_{\mathbf{k}}\{2\beta[A_0k^2 + A + 6B(g^2 + \mathcal{N}(g))]\}^{-1} \qquad (45)$$

then Eq. (35) gives for the free energy a function of g only, which reads

$$\frac{W}{\Omega} = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{\beta^{-1}}{2} + Ag^2 + Bg^4 - 3B\mathcal{N}^2(g)$$

$$- \frac{1}{2} \frac{\beta^{-1}}{\Omega} \sum_{\mathbf{k}} \log\{2\beta[A_0 k^2 + A + 6B(g^2 + \mathcal{N}(g))]\}^{-1} \qquad (46)$$

Equation (46) gives the value of the free energy along a locus of points on the hypersurface which goes through the equilibrium states of the systems.

In Figs. 4 and 5 we have plotted the free energy as a function of the order parameter for various values of ϵ for the values 1 and 0.1 of the parameter r/R. At low temperature the free energy has a pronounced minimum at the equilibrium value of the order parameter. From Eq. (41) one sees that the equilibrium value of the dimensionless order parameter $u = (4Br^2/A_0)^{1/2} g$ coincides with the value of the dimensionless inverse correlation length $r\xi^{-1}$. In other words the value of u at which the minimum of the free energy occurs coincides with the solution of Eq. (44).

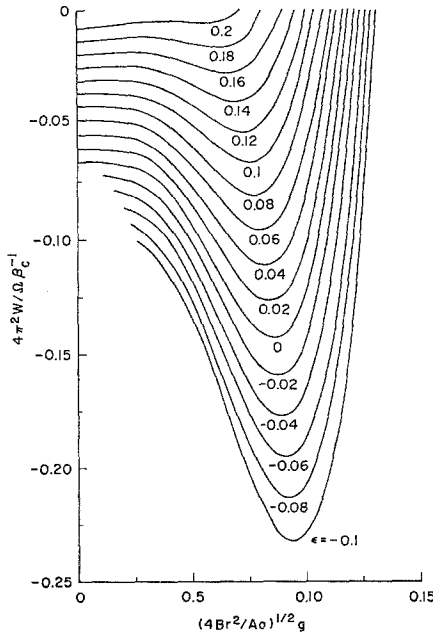Thus as the temperature is raised ξ^{-1} (or g) decreases; however, the

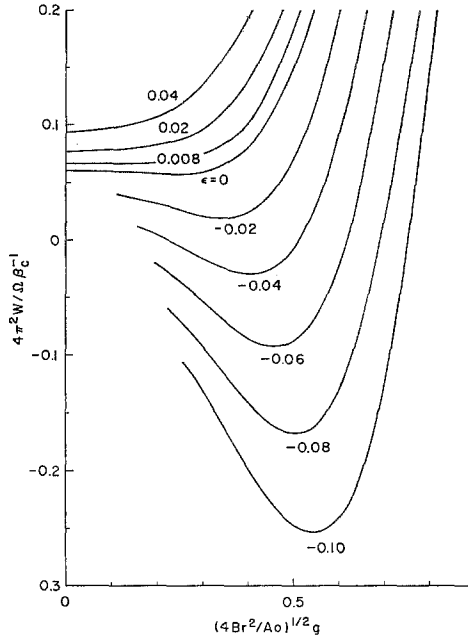Fig. 4.   Free energy vs. order parameter for $r/R = 1$.

Fig. 5.   Free energy vs. order parameter for $r/R = 0.1$.

minimum does not tend to zero as ϵ vanishes. By contrast, at $\epsilon = 0$ the equilibrium value of ξ^{-1} (or g) is nonzero. Furthermore, the extremal point at the origin, which corresponds to the solution $g = 0$ of Eq. (18) for $\mu = 0$, at $\epsilon = 0$ shifts from a maximum to a minimum. This corresponds to the onset at $\epsilon = 0$ of the new solution $\xi^{-1} = 0$ of Eq. (44). This new solution persists for $\epsilon > 0$ and corresponds to a local maximum of the free energy; therefore it must be discarded on grounds of thermodynamic stability. This maximum eventually merges with the minimum corresponding to the stable solution, producing an inflection point.

The transition occurs at the temperature $\epsilon^* > 0$ at which the two minima of the free energy have the same value. For $r/R = 1$ one has $\epsilon^* = 0.18$ and for $r/R = 0.1$, $\epsilon^* = 0.008$. Clearly, it is a first-order transition (Fig. 6).

Finally we compute the specific heat in the ordered phase. The equilibrium expression for the free energy

$$W = \sum_{\mathbf{k}} \frac{\beta^{-1}}{2} + \Omega \left(-\frac{A}{2B} + 6B\mathcal{N}^2 \right) - \frac{1}{2} \beta^{-1} \sum_{\mathbf{k}} \log q(\mathbf{k}) \qquad (47)$$

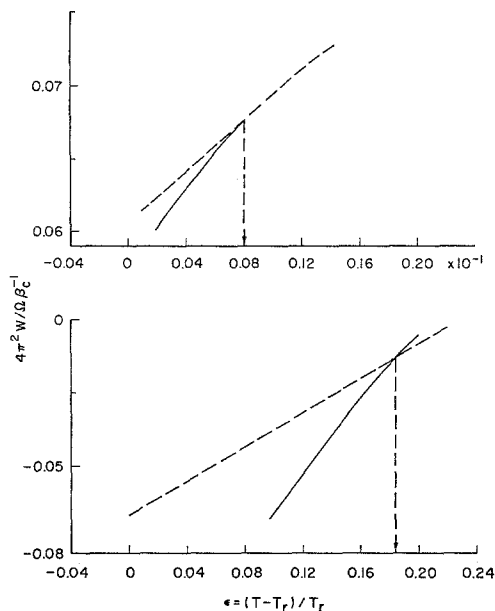is obtained by inserting Eqs. (41)–(43) into Eq. (35).

Fig. 6. Gibbs plots for the free energy for $r/R = 0.1$ (top) and $r/R = 1$ (bottom). The dashed line indicates the value of the free energy at the origin ($g = 0$) and the continuous line indicates the value of the free energy at the minimum $g \neq 0$.

The entropy and the specific heat are then given by

$$S = \Omega \left(\frac{A}{2B} - 2\mathcal{N} \right) \frac{\partial A}{\partial T} + \frac{k_B}{2} \sum_{\mathbf{k}} \log q(\mathbf{k}) \tag{48}$$

$$C = \sum_{\mathbf{k}} \frac{k_B}{2} + 2\Omega \left[\frac{\alpha^2 T}{4B} + \alpha\mathcal{N} + (A + 6B\mathcal{N}) \frac{\partial \mathcal{N}}{\partial T} + \alpha T_c \frac{\partial \mathcal{N}}{\partial T} \right] \tag{49}$$

The specific heat per unit volume in the ordered phase is plotted together with the classical contribution $(\Omega r^{-3}k_B/12\pi^2) + (\Omega\alpha^2 T/2B)$ in Fig. 2.

7. DISCUSSION

We shall first derive a validity criterion for the approximation. This is readily obtained extending to the present case the dimensional considerations of Ref. 10.

In the disordered phase an nth-order diagram for the self energy con-

tains $2n - 1$ q-lines. In the limit in which the self-consistent Hartree approximation is valid one can estimate the nth-order contribution to M by

$$M^{(n)} \propto (\beta B)^n \int d\mathbf{x}_1 \cdots d\mathbf{x}_{n-1} \, q^{2n-1} \tag{50}$$

where q is a Hartree correlation function. In coordinate spaces one has $q(\mathbf{r}) \propto e^{-r/\xi}/\beta A_0 r$. Thus for $r < \xi$ one can approximate the correlation function by $(\beta A_0 r)^{-1}$ and the order of magnitude of $M^{(n)}$ is given by

$$M^{(n)} \propto (B\beta)^n \, \xi^{n-2}/(\beta A_0)^{2n-1} \tag{51}$$

Comparing with Eq. (27)

$$M^{(n)} \propto 2\beta A_0 \xi^{-2}(\xi/R)^n \tag{52}$$

Since in the Hartree approximation $q^{-1}(\mathbf{k} = 0) = 2\beta A_0 \xi^{-2}$, we see from Eq. (52) that higher-order contributions to the self-energy are negligible for $\xi/R < 1$. Using Eq. (32), we can express the criterion of validity as a condition on the temperature, namely

$$\epsilon > \frac{\pi}{2} \frac{(r/R)^2}{1 + (r/R)} \tag{53}$$

If we compare with the condition for the validity of the classical theory $\xi_0/R < 1$, which gives

$$(T - T_c)/T_c > (r/R)^2 \tag{54}$$

we find no significant improvement, since $r/R \leqslant 1$.

We note that the criterion for the validity of the approximation is modified if one allows for a vector order parameter. In particular, in the limit of an infinite number of components the approximation becomes exact and gives the spherical model.[18,19,20]

In the case of an n-component vector field the coupling constant is replaced by B/n. Each closed loop contains a sum over the field components and thus carries a factor n. The argument is that for large n the dominant diagrams in any given order are those that contain the maximum number of closed loops, namely the bubble diagrams. An nth-order bubble diagram contains $n - 1$ loops; therefore is goes like $1/n$. In the limit $n \to \infty$ (spherical model) the only term which survives is the Hartree term.

Returning to the scalar field, in the ordered phase we arrive at the same result as in the disordered phase. The evaluation of the terms that do not contain the order parameter is unaltered. For those terms that do contain the order parameter we note that order parameter lines occur in pairs which

can be regarded as resulting from cutting open one q-line. Thus an nth-order diagram with two g-lines contains $2n - 2$ q-lines; consequently,

$$M^{(n)} \propto (\beta B)^n \int dx_1 \cdots dx_{n-1} \, g^2 q^{2n-2} \tag{55}$$

At equilibrium we have $g^2 = (A_0/4B)\,\xi^{-2}$; therefore

$$M^{(n)} \propto (\beta B)^n \frac{A_0}{B} \frac{\xi^{n-3}}{(\beta A_0)^{2n-2}}$$

namely,

$$M^{(n)} \propto \beta A_0 \xi^{-2} (\xi/R)^{n-1} \tag{56}$$

Some of the results we have obtained in the Hartree approximation reduce to classical results in the limit $B \to 0$, or equivalently $R \to \infty$. For the correlation length this can be seen directly from Eqs. (25) and (44), or qualitatively from Fig. 3, where one can compare the behavior of ξ^{-1} for two different values of r/R to the classical counterpart ξ_0^{-1}.

The susceptibility, which is simply related to the correlation length by Eq. (33), also tends to its classical counterpart in the limit $R \to \infty$. Note, however, that there is no classical limit for the order parameter and the specific heat. We shall return to this point later.

From the behavior of the correlation length it seems that the first-order transition in the Hartree approximation becomes a second-order transition in the classical limit $R \to \infty$. This might be surprising because while the classical theory treats only the order parameter self-consistently and neglects entirely the order paramater fluctuations, the approximation we have considered treats self-consistently both the order parameter and the order parameter fluctuations. However, there is an important difference in the structure of the equations obtained in the two cases.

The order parameter, the correlation length, and the susceptibility of the classical theory can be obtained by inserting the following approximations to M and K in Eqs. (7) and (11)[1,9]:

$$K(1) = \quad \text{(diagram)} \quad = -4B(1234)\,g(2)\,g(3)\,g(4) \tag{57}$$

$$M(12) = \quad \text{(diagram)} \quad = -12\beta B(1234)\,g(3)\,g(4) \tag{58}$$

Given these expressions for M and K, it is not possible to construct a functional Φ of g and q that satisfies Eq. (14). Furthermore, the expression for the free energy we have obtained in Eq. (47) does not reduce to the Landau free energy in the limit $R \to \infty$, since this limit does not exist for the classical free energy in the ordered phase. This explains why the expression for the specific heat given in Eq. (49) does not have a classical limit for $R \to \infty$. One does not encounter this problem in taking the limit for the correlation length and the susceptibility because these quantities, contrary to the order parameter and the specific heat, have classical counterparts which are independent of B. A second important difference between the Hartree approximation and the classical theory related to the structure of M and K stems from the fact that the expressions given in Eqs. (57) and (58) satisfy the functional relation

$$M(12) = \beta \, \delta K(1)/\delta g(2) \tag{59}$$

Equation (59) is a property of the exact theory.[1]

An approximation which verifies Eq. (59) in quantum manybody theory leads to a gapless excitation spectrum.[6] In the present context Eq. (59) is a necessary and sufficient condition for the validity of the result of linear response theory

$$q(12) = \beta^{-1} \, \delta q(1)/\delta \mu(2) \tag{60}$$

in an approximate theory.[1]

By contrast, the self-energy and the effective field of the Hartree approximation, Eqs. (16) and (17), do not satisfy Eq. (59). In fact, from Eq. (16), one has

$$\beta \frac{\delta K(1)}{\delta g(2)} = \qquad \qquad + \qquad \qquad + \qquad \qquad \tag{61}$$

where the shaded bubble represents the sum of the terms coming from the variation of q with respect to g and is not present in Eq. (17). This term obviously disappears in the disordered phase, where the Hartree approximation is consistent with Eq. (59).

Although we will not attempt to prove it here, one can infer that the validity of Eq. (59) is required for an approximation to exibit a second-order phase transition. Namely, the existence of a singularity for the correlation function at $\mathbf{k} = 0$ and $T = T_r$ is related to the validity of Eq. (59) through an extension to finite temperatures and classical systems of the proof of the Pines–Hugenholtz theorem as given, for example in Ref. 6, Section 6.

APPENDIX A. FREE ENERGY, ENTROPY, AND SPECIFIC HEAT IN THE DISORDERED PHASE

With the form (3) for the couplings and the approximation (15) for Φ, Eq. (13) becomes

$$W\{g; q(\mathbf{k})\} = \Omega(-\mu g + Ag^2 + Bg^4) + \sum_{\mathbf{k}} (A + A_0 k^2) q(\mathbf{k})$$

$$+ 6Bg^2 \sum_{\mathbf{k}} q(\mathbf{k}) + \frac{3B}{\Omega} \sum_{\mathbf{k}\mathbf{k'}} q(\mathbf{k}) q(\mathbf{k'}) \tag{A.1}$$

$$- \frac{1}{2} \beta^{-1} \sum_{\mathbf{k}} \log q(\mathbf{k})$$

In the disordered phase, $g = 0$, and for $q(\mathbf{k})$ satisfying Eq. (21), Eq. (A.1) reduces to

$$W\{q(\mathbf{k})\} = \sum_{\mathbf{k}} \tfrac{1}{2}\beta^{-1} - 3B\Omega\mathcal{N}^2 - \tfrac{1}{2}\beta^{-1} \sum_{\mathbf{k}} \log q(\mathbf{k}) \tag{A.2}$$

Differentiating with respect to the temperature, we obtain the entropy:

$$S = -\frac{\partial W}{\partial T} = -\sum_{\mathbf{k}} \frac{k_B}{2} + 6B\Omega\mathcal{N} \frac{\partial\mathcal{N}}{\partial T} + \frac{k_B}{2} \sum_{\mathbf{k}} \log q(\mathbf{k})$$

$$+ \frac{1}{2} \beta^{-1} \sum_{\mathbf{k}} q^{-1}(\mathbf{k}) \frac{\partial q(\mathbf{k})}{\partial T} \tag{A.3}$$

Furthermore, from Eq. (21),

$$\frac{\partial q(\mathbf{k})}{\partial T} = \frac{1}{T} q(\mathbf{k}) - 2\beta \left[\frac{\partial A}{\partial T} + 6B \frac{\partial\mathcal{N}}{\partial T} \right] q^2(\mathbf{k}) \tag{A.4}$$

Thus, inserting in Eq. (A.3), we obtain

$$S = -\Omega \frac{\partial A}{\partial T} \mathcal{N} + \frac{k_B}{2} \sum_{\mathbf{k}} \log q(\mathbf{k}) \tag{A.5}$$

Differentiating once more with respect to the temperature, we obtain the specific heat

$$C = T \frac{\partial S}{\partial T} = -\Omega T \frac{\partial^2 A}{\partial T^2} \mathcal{N} - \Omega T \frac{\partial A}{\partial T} \frac{\partial\mathcal{N}}{\partial T} + T \frac{k_B}{2} \sum_{\mathbf{k}} q^{-1}(\mathbf{k}) \frac{\partial q(\mathbf{k})}{\partial T}$$

Using Eq. (A.4) and $A = \alpha(T - T_c)$, the above result reduces to

$$C = \sum_{\mathbf{k}} \frac{k_B}{2} - \Omega\alpha\mathcal{N} - \Omega(A + 6B\mathcal{N}) \frac{\partial\mathcal{N}}{\partial T} - \Omega\alpha T_c \frac{\partial\mathcal{N}}{\partial T} \tag{A.6}$$

The temperature dependence of $\mathcal{N}$ for small ϵ is obtained from Eqs. (24 and 32), i.e.,

$$\mathcal{N} = \frac{A_0}{6B} \left(\xi^{-2} - \xi_0^{-2} \right)$$

with

$$\xi^{-2} = \frac{A + 6B\mathcal{N}}{A_0} \cong r^{-2} \left[\frac{2}{\pi} (a + b) \right]^2 \epsilon^2; \qquad a = \frac{R}{r}, \quad b = r\bar{p}$$

Inserting in Eq. (A.6), we obtain

$$C = \sum_{\mathbf{k}} \frac{k_B}{2} + k_B \frac{\Omega r^{-3}}{4\pi^2} \left\{ \frac{a^2}{a + b} + \left[\frac{a^2}{a + b} - \frac{8}{\pi^2} (a + b)^3 \right] \epsilon \right.$$

$$\left. - 2 \left(\frac{2}{\pi} \right)^4 (a + b)^5 \, \epsilon^3 \right\} \tag{A.7}$$

APPENDIX B

In the limit $B \to 0$ the fluctuations are given by

$$\mathcal{N}_0 = \frac{1}{\Omega} \sum_{\mathbf{k}} q_0(\mathbf{k}) = \frac{1}{4\pi^2 \beta A_0} \int_0^{\bar{p}} d\mathbf{k} \, \frac{k^2}{k^2 + \xi_0^{-2}} \tag{B.1}$$

This gives

$$\mathcal{N}_0 = \frac{\bar{p}}{4\pi^2 \beta A_0} - \frac{\xi_0^{-1}}{4\pi^2 \beta A_0} \tan^{-1} \left(\frac{\bar{p}}{\xi_0^{-1}} \right)$$

In the neighborhood of the transition

$$\mathcal{N}_0 \cong \frac{\bar{p}}{4\pi^2 \beta A_0} - \frac{\xi_0^{-1}}{8\pi \beta A_0} \tag{B.2}$$

Thus the dominant term in the temperature derivative is given by

$$\frac{\partial \mathcal{N}_0}{\partial T} \cong \frac{1}{16\pi \beta A_0} \left(\frac{\alpha}{A_0} \right)^{1/2} (T - T_c)^{-1/2} \tag{B.3}$$

Inserting Eqs. (B.2) and (B.3) in Eq. (A.6), we see that in the limit $B = 0$ the specific heat diverges as $[(T - T_c)/T_c]^{-1/2}$ when $T \to T_c$.

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