Self-Consistent Treatment of a Phase Transition in a System with a Vector Order Parameter

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The problem of the continuation of the Hartree approximation below the transition temperature is considered for a system with a vector order parameter. In contrast to the case of a scalar order parameter, considered in a previous paper, it is found that a self-consistent and gapless approximation can be constructed in the limit of a very large number of vector components. The results agree with those of the spherical model.

1. INTRODUCTION

Self-consistent approximations of the Hartree type have been applied by various authors[1] to the study of the superconducting transition and by Murata and Doniach[2] to the phase transition in itinerant ferromagnets.

In a previous paper[3] we considered the problem of the continuation of the Hartree approximation below T_c in an arbitrary system described by a scalar order parameter.

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The main results of this paper were as follows.

(a) We obtained a set of critical exponents as T_c is approached from above ($\gamma = 2$, $\nu = 1$, $\alpha = -1$).

(b) When the decoupling of the order parameter correlation function characteristic of the Hartree approximation is imposed below T_c, thermodynamic equilibrium requirements lead to a shift of the transition temperature and the transition becomes of first order.

(c) These features of the approximation below T_c are ascribed to a violation of the condition of gaplessness. On the other hand, a gapless continuation to the ordered phase of the Hartree approximation cannot be performed in the case of a scalar order parameter.

It has recently been realized[4,5] that for $T > T_c$ the Hartree approximation becomes exact for a system with a vector order parameter in the limit of a very large number of components. In fact it reproduces the results of the spherical model.[6] We expect that in this limit the description of the ordered phase ($T < T_c$) will also be greatly simplified. This is indeed the case and in this paper we consider a soluble self-consistent approximation which becomes exact when m, the number of vector components, tends to infinity.

Although the results reported are not new[2] (Brezin and Wallace[5] have in fact computed the exponent β to order $1/m$), it is of interest to show how in the framework of the $1/m$ expansion a gapless and self-consistent continuation of the Hartree approximation arises in a natural way.

2. BASIC EQUATIONS

We represent the partition function of the system by a functional integral[7]

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

where $F\{\boldsymbol{\eta}(\mathbf{x})\}$ is the Landau–Ginzburg functional for a vector order parameter $\boldsymbol{\eta}(\mathbf{x}) = [\eta_1(\mathbf{x}),..., \eta_m(\mathbf{x})]$:

$$F\{\boldsymbol{\eta}(\mathbf{x})\}/K_B T = \int d^d x \,\{\tfrac{1}{2}\nabla\boldsymbol{\eta}\cdot\nabla\boldsymbol{\eta} + \tfrac{1}{2}A\boldsymbol{\eta}(\mathbf{x})\cdot\boldsymbol{\eta}(\mathbf{x})$$
$$+ B[\boldsymbol{\eta}(\mathbf{x})\cdot\boldsymbol{\eta}(\mathbf{x})]^2 - \mu\eta_1(\mathbf{x})\} \tag{2}$$

In Eq. (2) K_B is the Boltzmann constant, d is the dimensionality of the

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[2] Results similar to those contained in this paper have been obtained by S. Ma (Univ. of California—La Jolla preprint) in his analysis of the renormalization group in the large-m limit. This work came to our attention after the completion of this paper.

system, A depends linearly on the temperature, B is a positive constant of order $1/m$ to ensure $\log Z \propto m$, and μ is an external field in the direction of the vector component number one.

The external field μ breaks the spherical symmetry and a nonzero expectation value for $\eta_1(\mathbf{x})$ results, i.e.,

$$g = \langle \eta_1(\mathbf{x}) \rangle \neq 0 \tag{3}$$

which is independent of $\mathbf{x}$ for a translationally invariant system. The angular bracket denotes thermodynamic average.

We introduce the new field

$$\psi(\mathbf{x}) = \eta_1(\mathbf{x}) - g \tag{4}$$

and rewrite Eq. (2) as

$$
\begin{aligned}
(K_B T)^{-1} & F\{g, \psi, \eta_2 \cdots \eta_m\} \\
= & \ \Omega[\tfrac{1}{2}Ag^2 + Bg^4 - \mu g] + \int d^d x \ \{\tfrac{1}{2}(\nabla\psi)^2 + \tfrac{1}{2}A\psi^2(\mathbf{x}) \\
& + \tfrac{1}{2} \sum_{j=2}^{m} [(\nabla\eta_j)^2 + A\eta_j{}^2(\mathbf{x})] + 6Bg^2\psi^2(\mathbf{x}) + 2Bg^2 \sum_{j=2}^{m} \eta_j{}^2(\mathbf{x}) \\
& + B\left[\psi^2(\mathbf{x}) + \sum_{j=2}^{m} \eta_j{}^2(\mathbf{x})\right]^2 + 4Bg\psi(\mathbf{x})\left[\psi^2(\mathbf{x}) + \sum_{j=2}^{m} \eta_j{}^2(\mathbf{x})\right] \\
& + [(A + 4Bg^2)g - \mu]\psi(\mathbf{x})\}
\end{aligned}
\tag{5}
$$

where Ω is the volume of the system.

The quantities of interest are the average order parameter g, and the transverse and the longitudinal correlation functions defined, respectively, by

$$
\begin{aligned}
q_T(\mathbf{x} - \mathbf{x}') &= \langle \eta_j(\mathbf{x})\eta_j(\mathbf{x}') \rangle, \qquad j = 2,...,m \\
q_L(\mathbf{x} - \mathbf{x}') &= \langle \psi(\mathbf{x})\psi(\mathbf{x}') \rangle.
\end{aligned}
\tag{6}
$$

In the following we shall consider the Fourier transform of the correlation functions $q_{T,L}(\mathbf{k}) = \int d^d x \ q_{T,L}(\mathbf{x}) \exp(i\mathbf{k}\cdot\mathbf{x})$. We can formally write down a closed set of equations[7]

$$q_0{}^{-1}(\mathbf{k} = 0)g = \mu + \mathrm{K} \tag{7}$$

$$q_T{}^{-1}(\mathbf{k}) = q_0{}^{-1}(\mathbf{k}) - M_T{}^{-1}(\mathbf{k}) \tag{8}$$

$$q_L{}^{-1}(\mathbf{k}) = q_0{}^{-1}(\mathbf{k}) - M_L(\mathbf{k}) \tag{9}$$

where $q_0{}^{-1}(\mathbf{k})$ is defined by

$$q_0{}^{-1}(\mathbf{k}) = k^2 + A \tag{10}$$

and K, M_T, M_L are functionals of g, q_T, q_L.

The set of equations (7)–(9) is obtained by generalizing[3] to the case of a vector order parameter the formalism developed in Ref. 7 for the case of a scalar field. In the same way one can also derive an expression for the dimensionless free energy as a functional of g, q_T, q_L:

$$W\{g, q_T, q_L\} = \Omega[\tfrac{1}{2}Ag^2 - \mu g] + \tfrac{1}{2}\sum_{\mathbf{k}} q_0^{-1}(\mathbf{k})q_L(\mathbf{k}) + \tfrac{1}{2}m\sum_{\mathbf{k}} q_0^{-1}(\mathbf{k})q_T(\mathbf{k})$$

$$- \tfrac{1}{2}\sum_{\mathbf{k}}\log q_L(\mathbf{k}) - \tfrac{1}{2}m\sum_{\mathbf{k}}\log q_T(\mathbf{k}) - \tfrac{1}{2}\Phi\{g, q_T, q_L\} \quad (11)$$

where the functional Φ, in the exact theory and in any approximation giving consistent thermodynamics,[8] is related to the quantities K, M_T, M_L entering Eqs. (7)–(9) by

$$\left(\frac{\delta\Phi}{\delta g}\right)_{q_T, q_L} = 2K, \qquad \left(\frac{\delta\Phi}{\delta q_L(\mathbf{k})}\right)_{g, q_T} = M_L(\mathbf{k}), \qquad \left(\frac{\delta\Phi}{\delta q_T(\mathbf{k})}\right)_{g, q_L} = M_T(\mathbf{k}) \quad (12)$$

In addition, the above expression for the free energy has the variational property[7] that it is stationary around the equilibrium values of its arguments. Namely, the stationarity condition

$$(\delta W/\delta g)_{q_T, q_L} = 0 \tag{13}$$

$$(\delta W/\delta q_T(\mathbf{k}))_{g, q_L} = 0 \tag{14}$$

$$(\delta W/\delta q_L(\mathbf{k}))_{g, q_T} = 0 \tag{15}$$

is equivalent to the set of (7)–(9).

3. THE LARGE m LIMIT

In computing orders of magnitude, we take into account that $B \sim 1/m$, $g \sim m^{1/2}$, as can be verified by inserting the first contribution to $K \sim Bg^3$ in Eq. (7), and that each transverse loop contributes a factor m.

The lowest-order contributions in the skeleton expansions of K, M_T, M_L can then be represented by the diagrams

$$\mathsf{K} = \qquad + \qquad + \; 0(m^{-1/2}) \tag{16}$$

$$\mathsf{M_T} = \qquad + \qquad + \; 0(\tfrac{1}{m}) \tag{17}$$

[3] The details of the formalism for the case of a vector order parameter will be presented elsewhere.

$$M_L = \quad \text{(diagram)} \quad + \quad \text{(diagram)} \quad + \quad \text{(diagram)} \quad + O(\tfrac{1}{m}) \tag{18}$$

where the dot represents the coupling constant B, the wavy line represents the order parameter g, the dashed line represents the transverse correlation function q_T, and the shaded bubble represents the sum of strings of bubbles, namely:

$$\text{(diagram)} = \text{(diagram)} + \text{(diagram)} + \text{(diagram)} + \cdots \tag{19}$$

The transverse self-energy M_T does not include bubble terms, since one of the internal lines must be longitudinal and the other must have the same vector index as the external lines. This precludes summation over the vector components and the contribution is of order $1/m$.

In order to have an expression for the free energy consistent with the approximation defined by Eqs. (16)–(18), in Eq. (11) we must retain the contribution to Φ represented by the diagrams

$$\Phi = \quad \text{(diagram)} + \text{(diagram)} + \text{(diagram)} + \text{(diagram)} + \text{(diagram)} + \text{(diagram)} \tag{20}$$

where the continuous line represents q_L. The set of equations (16)–(18) and (20) is consistent with Eqs. (12).

Next we note that the only correlation functions entering Eqs. (16)–(18) are transverse and that the transverse self-energy is of Hartree type. Therefore we can solve Eqs. (7)–(9) self-consistently. Defining

$$N = (1/\Omega) \sum_{\mathbf{k}} q_T(\mathbf{k}) \tag{21}$$

$$S(\mathbf{k}) = (1/\Omega) \sum_{\mathbf{p}} q_T(\mathbf{p} - \mathbf{k}) q_T(\mathbf{p}) \tag{22}$$

$$\Gamma(\mathbf{k}) = 4mBS(\mathbf{k})/[1 + 4mBS(\mathbf{k})] \tag{23}$$

we can write the basic equations as

$$Ag = \mu - 4Bg^3 - 4mBNg \tag{24}$$

$$q_T^{-1}(\mathbf{k}) = k^2 + A + 4Bg^2 + 4mBN \tag{25}$$

$$q_L^{-1}(\mathbf{k}) = k^2 + A + 12Bg^2 + 4mBN - 8g^2B\Gamma(\mathbf{k}) \tag{26}$$

If $T > T_c$, then $\lim_{\mu \to 0} g = 0$ and any distinction between longitudinal and transverse modes disappears. From Eqs. (25) and (26) we get

$$q_T^{-1}(\mathbf{k}) = q_L^{-1}(\mathbf{k}) = k^2 + A + 4mBN \tag{27}$$

which is of the type analyzed in Ref. 3 and leads to the set of critical exponents $\gamma = 2$, $\nu = 1$, $\alpha = -1$. The transition temperature T_c is defined by the divergence of the susceptibility

$$\chi^{-1} = q^{-1}(\mathbf{k} = 0, T_c) = 0 = A(T_c) + 4mBN(T_c) \qquad (28)$$

If $T < T_c$, then $\lim_{\mu \to 0} \mu/g = 0$. Let us first look at the inverse susceptibilities. From Eqs. (24) and (25) it is trivial to verify that

$$q_T^{-1}(\mathbf{k} = 0) = \mu/g \qquad (29)$$

This exact relation holds in any approximation which satisfies $\mathrm{K} = gM_T(\mathbf{k} = 0)$.[9] Furthermore, from Eq. (26), to lowest order in μ/g, one has

$$q_L^{-1}(\mathbf{k} = 0) = (8\pi/m)g^2(\mu/g)^{\varepsilon/2} \qquad (30)$$

where $\epsilon = 4 - d$ and $2 < d < 4$, in agreement with the result of Brezin and Wallace.[5]

From Eqs. (21) and (29) for $d = 3$ we have

$$N = N(T_c) - (1/4\pi)(\mu/g)^{1/2} \qquad (31)$$

Inserting this result in Eq. (24), we obtain the equation of state

$$\left(\frac{m}{16\pi B}\right)^2 \frac{\mu}{g^\delta} = \left[\frac{A - A(T_c)}{4Bg^{1/\beta}} + 1\right]^\gamma \qquad (32)$$

with $\gamma = 2$, $\beta = \frac{1}{2}$, $\delta = 5$.

In order to show that Eq. (28) defines the transition temperature unambiguously, we shall now consider the behavior of the order parameter.

From Eqs. (29) and (30) one sees that when $\mu \to 0$ both susceptibilities diverge for $T < T_c$. Consequently, in order to define the transition temperature within the approximation considered for the ordered phase, we cannot look at the divergence of the susceptibility and we must consider the order parameter.

Let us set $\mu = 0$. Then from Eqs. (21) and (29) it follows that $N = N(T_c)$ for all $T < T_c$. Using Eq. (28), we may then write Eq. (24) as

$$4Bg^2 = A(T_c) - A \qquad (33)$$

which implies $\beta = \frac{1}{2}$ and proves that the temperature at which the order parameter vanishes is indeed given by T_c.

This result shows that the approximation defined by Eqs. (16)–(18) solves the difficulty encountered in the case of a scalar field which we mentioned in point (b) of the introduction. With regard to this we note that in the present approximation K and M_L satisfy a relation of the exact theory, usually referred to as condition of gaplessness,[8] which was violated

in the approximation considered in Ref. 3. This point will be considered in more detail in the next section.

4. GAPLESSNESS, STABILITY, AND SPECIFIC HEAT

The condition of gaplessness, when translational invariance holds, is expressed as

$$M_L(\mathbf{k} = 0) = \delta K/\delta g \tag{34}$$

We must therefore check that the diagrams for M_L are obtained by differentiating K with respect to g. K depends on g explicitly and implicitly through q_T. Differentiation with respect to the explicit dependence generates the first two diagrams in Eq. (18). Next we consider the loop and we note that

$$\frac{\delta}{\delta g} \; \bigcirc \;\; = \;\; \mathrel{\mathbf{\triangleright}} \tag{35}$$

where the three-point vertex is given by

$$\mathrel{\mathbf{\triangleright}} \; = \; \frac{\delta g_T^{-1}}{\delta g} \tag{36}$$

Differentiating Eq. (25) and solving by iteration, one finds

$$\mathrel{\mathbf{\triangleright}} \; = \; 2 \left[\; 4 \; \bigcirc \; - \; (4)^2 \; \bigcirc\!\bigcirc \; + \; (4)^3 \; \bigcirc\!\bigcirc\!\bigcirc \; + \; .... \right] \tag{37}$$

Inserting this result into Eq. (35), we obtain the sum of bubbles appearing in Eq. (18), which completes the proof that M_L and K satisfy the condition of gaplessness.

Let us now consider the thermodynamic stability of the solution for the order parameter in the ordered phase. We note that for $T < T_c$ and $\mu = 0$ Eq. (24) also admits the solution $g = 0$. Using the variational property of the free energy, one can verify that the nontrivial solution considered above actually minimizes the free energy up to T_c. We shall denote by g_0 and g_1, respectively, the trivial and the nontrivial solution.

Regarding the free energy as a functional of the order parameter only, we have

$$\frac{\delta W}{\delta g} = \left(\frac{\delta W}{\delta g}\right)_{q_L, q_T} + \left(\frac{\delta W}{\delta q_T}\right)_{g, q_L} \frac{\delta q_T}{\delta g} + \left(\frac{\delta W}{\delta q_L}\right)_{g, q_T} \frac{\delta q_L}{\delta g} \tag{38}$$

The dependence of q_T and q_L on the order parameter is given by Eqs. (25) and (26). In other words, one varies the order parameter and takes the correlation functions to have the equilibrium expressions consistent with the

given values of g. Thus, by virtue of Eqs. (14) and (15) the last two terms on the r.h.s. of Eq. (38) vanish, and one has

$$\delta W/\delta g = Ag - \text{K} \tag{39}$$

which shows that g_0 and g_1 are extremal points of W.

By a similar argument, the second derivative gives

$$\delta^2 W/\delta g^2 = A - M_L(\mathbf{k} = 0)$$

where we have used the property of gaplessness of the approximation.

From the structure of M_L it follows that

$$(\delta^2 W/\delta g^2)_{g=g_0} = A - 4mBN(T_c) = A - A(T_c) < 0 \tag{40}$$

$$(\delta^2 W/\delta g^2)_{g=g_1} = q_L{}^{-1}(\mathbf{k} = 0) = 0 \tag{41}$$

The result (40) is sufficient to conclude that the extremal point at g_1 must be a minimum for all $T < T_c$.

It is worth noticing that in the Hartree-type approximation that we have analyzed in Ref. 3 for the case of a scalar order parameter, g_1 minimizes the free energy up to a temperature $T^* > T_c$. At $T = T^*$ a first-order transition occurs and g_0 minimizes the free energy for $T > T^*$.

We conclude this section by considering the specific heat. For the computation we need the explicit expression for the free energy density to lowest order in $1/m$, namely

$$\frac{W}{\Omega} = -\mu g + \frac{A}{2} g^2 + Bg^4 + \frac{m}{2\Omega} \sum_{\mathbf{k}} [q_0{}^{-1}(\mathbf{k}) + 4Bg^2 + 2mBN]q_T(\mathbf{k})$$

$$-\frac{m}{2\Omega} \sum_{\mathbf{k}} \log q_T(\mathbf{k}) + O(1) \tag{42}$$

Using Eq. (25), this reduces to

$$\frac{W}{\Omega} = -\mu g + \frac{A}{2} g^2 + Bg^4 - m^2 BN^2 - \frac{m}{2\Omega} \sum_{\mathbf{k}} \log q_T(\mathbf{k}) \tag{43}$$

Setting $\mu = 0$ and $T > T_c$, in three dimensions Eq. (43) leads to the result[3]

$$\frac{c}{\Omega} = \frac{1}{8B}\left\{1 - \frac{2[A - A(T_c)]}{(2m\pi B)^2}\right\} \tag{44}$$

For $T < T_c$ the temperature dependence is contained only in the order parameter and we get

$$c/\Omega = 1/8B \tag{45}$$

for all $T < T_c$.

In conclusion, by considering the lowest-order contributions to the quantities K, M_T, M_L in the $1/m$ expansion, we have found an approximation which describes the continuation to the ordered phase of the Hartree approximation. The results are in agreement with those of the spherical model. The point of interest is that the $1/m$ expansion provides a useful framework for the construction of a self-consistent approximation valid on both sides of the transition.

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