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Field Theory Description of Continuous Phase Transitions[1]

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We present a formalism of a scalar, classical, and time-independent field theory of the type proposed by Ferrell for the treatment of continuous phase transitions. The formalism is developed along lines similar to those of many-body theory. All physical quantities, e.g., susceptibility, correlation length, and free energy, are expressed as functionals of the two-point time-independent correlation function and the order parameter. This is done both in the ordered and in the disordered phase. We obtain renormalized equations and diagram expansions of all quantities and self-consistent approximation schemes are presented. It is shown that near the transition temperature, which is defined within the theory, no weak coupling limit exists. The generalization to more complicated field symmetries is straightforward.

KEY WORDS: Phase transition; field theory; order parameter; renormalization; approximation schemes.

1. INTRODUCTION

In recent attempts to break beyond classical theories for general continuous phase transitions it was suggested that the most important ingredients are the long-wavelength spatial variation of the order parameter. One approach was to postulate a statistical mechanics in terms of a spatially varying field.

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The field is defined on a coarse-grained space so that: (a) the field becomes classical due to averaging over a cell and (b) effects stemming from variations on a scale smaller than the size of a cell are assumed unimportant.[1-3]

In this approach the statistical mechanics is prescribed by postulating a weight for each distribution of the field. More specifically, if $\eta(\mathbf{x})$ is a scalar field, then one writes the weight as

$$w\{\eta(\mathbf{x})\} = \exp[-\beta F\{\eta(\mathbf{x})\}] \tag{1}$$

where

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

where s is the number of dimensions. The partition function is obtained by summing over all possible distributions $\eta(\mathbf{x})$ assuming all other variables to have been summed previously.

In the above A_0, A, and B are constants whose values are not determined within the theory. They are in principle calculated from the microscopic theory in coarse-graining and in the elimination of short-range phenomena. Explicit calculation of the coefficients is beyond the power of present techniques. However, the qualitative nature of the transition is assumed to be independent of their particular values. They can, of course, be determined from experiment.

On the other hand, direct assaults on the various many-body Hamiltonians have been carried out.[4-6] The dependence of correlation functions on high momentum is eliminated and it is argued that only zero-frequency quantities are important. The parameters of the problem, renormalized by the above considerations, are again beyond the power of calculation and eventually the equations for the correlation functions and the dependence, near the transition, of various physical quantities on the correlation functions are essentially the same as in the model of Eq. (2).

Both Ferrell[1] and Migdal and Polyakov[4,5] claim that their respective results for the thermodynamics of the system obey scaling relations between the critical exponents.[6] This clearly goes beyond the classical theory[7] and gives a theory which treats its own fluctuations. This should apply all the way to the critical point.

The same problem was recently treated by Wilson[8a-8c] using the technique of the renormalization group to qualitatively calculate the critical exponents. The latter turn out to have nonclassical values.

In the present paper we develop the formalism of a theory based on Eq. (2). First we motivate the form of Eq. (2) and explain our notion of the order parameter. Then we consider the classical theory as an approximation to the present model and discuss critically the relations obtained in the classical theory between thermodynamic quantities and the correlation function.

Following these preliminaries, we turn to a study of the full implications of our postulated statistical mechanics. We do this along lines similar to Martin and Schwinger,[9] Baym,[10] and De Dominicis and Martin[11] and eventually arrive at: (a) the equation of "motion" for the correlation function, (b) the expression for the correlation function in terms of a "mass operator," (c) the self-consistent approximation schemes, and (d) the expression for the free energy in terms of the order parameter correlation function. The free energy is stationary with respect to variations of the order parameter and correlation function and thus it can be used for variational calculations of these quantities.

The discussion of results is deferred to future communications. Generally speaking, we feel that the present approach is complementary to that of Wilson, and a unification of the two may prove very fruitful.

2. NATURE OF THE ORDER PARAMETER

A general feature of continuous phase transitions is the anomalous behavior of certain thermodynamic and response functions; examples are the divergence of the susceptibility for a magnetic system and the divergence of the compressibility at the critical point of a liquid–gas system. These are the most divergent quantities.

This indicates that at the transition the system is in a regime dominated by large fluctuations with long-range correlations. In fact, from linear response theory the susceptibility $\chi = (\partial\langle\eta\rangle/\partial\mu)_{\mu=0}$ of the average bulk order parameter $\langle\eta\rangle$ with respect to an external disturbance μ is related to the order parameter correlation function $\langle\eta(\mathbf{x})\,\eta(\mathbf{x}^1)\rangle = g(\mathbf{x}-\mathbf{x}^1)$, where the angular brackets denote ensemble average by

$$\chi = \beta\int_{\Omega} d^d r\, g(\mathbf{r}); \qquad \beta^{-1} = k_B T, \qquad \mathbf{r} = \mathbf{x} - \mathbf{x}' \tag{3}$$

Thus, as the transition is approached the range of the correlation function must increase in order for the integral to be divergent at infinity. Therefore, configurations of the system which are spatially nonuniform may be expected to contribute significantly to the free energy.

The free energy for nonuniform systems can be represented by the integral over the volume of the system of a free energy density[12]:

$$F = \int_{\Omega} d^d x\, F(\mathbf{x})$$

In order to construct $F(\mathbf{x})$, we divide the volume Ω of the system into cells whose volume is small compared to Ω but large enough that a local order parameter can be defined as a classical field by averaging over the volume of the cell some corresponding microscopic observable.[13,14]

To elucidate this point, we recall that the concept of order parameter plays a central role in the phenomenological theory of continuous transitions.[15] It is a quantity that vanishes "above" and is nonzero "below" the transition; in other words, the numerical value of the order parameter is an indication of the degree of ordering of the system.

At the more fundamental level of the quantum many-body description of the system the appearance of a nonzero value of the order parameter in the absence of an external field is a manifestation of spontaneous symmetry breaking.[16,17]

It is a general feature of many-body physics that, along with microscopic observables subjected to the laws of quantum mechanics, there exist properties of the system macroscopic in the sense that their changes obey classical laws.[9,17] To say this differently, to each value of an observable to be regarded as macroscopic there corresponds a set of states distinguished only by the values of microscopic observables; the manifold of these states forms a Hilbert space and there is no interference between states belonging to Hilbert spaces associated with different values of the macroobservable.[17] A macroobservable is said to be invariant or noninvariant with respect to a group of transformations according to whether the associated Hilbert spaces are invariant or not under the transformations of the group. The order parameter belongs to the latter class; specifically, it is a macroscopic property of the system which is not invariant with respect to some group of symmetry transformations of the Hamiltonian. Here we will be concerned with a scalar field only but the results can be extended to fields with other symmetry groups.

Macroobservables are generally obtained as space averages of local microobservables [e.g., products of field operators $\psi(\mathbf{r}, t)$, $\psi^{\dagger}(\mathbf{r}, t)$] and the definition requires the limit of an infinite volume of integration.[17] This requirement cannot be exactly met when integrating over the finite volume of the cells, however; we choose the size of each cell large enough that on a microscopic scale it can be regarded as infinite to a good approximation and the resulting *local* macroscopic order parameter can be treated as a classical field. A rough scale for the coarse-graining will be the range of the interaction.

From now on we shall assume that the configurations of the system are described by an otherwise unspecified classical scalar field order parameter defined by

$$\eta(\mathbf{x}) = \omega^{-1} \int_{\omega} d^3y\, \hat{\eta}(\mathbf{y})$$

where $\hat{\eta}$ is the corresponding microscopic observable and ω is the volume of the cell centered at $\mathbf{x}$.

3. FREE ENERGY FUNCTIONAL

If on a microscopic scale the volume of the cell can be considered infinite, on the other hand, on a macroscopic scale it must be small so that the coarse-graining does not alter substantially the description of the phenomena of interest. Specifically, as suggested by the divergence of the static susceptibility, Eq. (2), only long-wavelength, long-range effects are expected to be important in the neighborhood of the transition. Hence the size of the cell must be small compared to the dominant wavelengths.

At a given temperature T and for a given value of the order parameter $\eta(\mathbf{x})$ the cell around $\mathbf{x}$ contributes to the total free energy the amount $\omega F(T, \eta(x))$. Since ω is finite and small, this quantity is analytic[13] both in T and η; we may then expand in power series and, dividing through by ω, we find for the free energy density

$$F(T, \eta(\mathbf{x})) = F_0(T) + A\eta^2(\mathbf{x}) + B\eta^4(\mathbf{x}) \tag{4}$$

with $A = \alpha(T - T_c)$, $\alpha > 0$, $B > 0$; T_c is a fixed temperature (see discussion in Section 8) and $F_0(T)$ represents the free energy density when $\eta = 0$, which we shall not explicitly consider from now on. None of the results in the present paper will depend on this particular choice of the coefficients. This form is suggestive and makes the relation of the model to previous calculations more explicit. For example, the Ising model of a magnet with infinite-range interaction leads to a free energy of the above form[13]: If J is the strength of the interaction, then the average energy is simply $E = -JM^2$, where M is the average magnetization and $J > 0$. From a combinatorial argument it can be shown that the entropy S, the logarithm of the number of states with a given M, has an expansion of the form $S(M) = aM^2 + bM^4 + \cdots$ with $a < 0$, $b < 0$.[a] Hence, the free energy is given by

$$F(T, M) = E - TS = -(J + aT)M^2 - TbM^4$$

If we now assume that the cells are independent of one another, then the free energy for a given distribution is given by

$$F\{\eta\} = \omega \sum_i F(\eta(\mathbf{x}_i)) = \omega \sum_i [A\eta^2(\mathbf{x}_i) + B\eta^4(\mathbf{x}_i)] \tag{5}$$

where the sum is extended over the cells and $\eta(\mathbf{x}_i)$ is the value of the order parameter at the ith cell in the considered distribution of the field.

[a] Such a model is sometimes referred to as the Kittel model, for which we have been unable to find the exact reference.

The partition function is then obtained by summing over all possible distributions

$$Z = \int_{-\infty}^{+\infty} \prod_i \frac{d\eta_i}{\epsilon(\omega)} \exp\left[-\beta\left(\omega \sum_i F(\eta_i)\right)\right] \tag{6}$$

where we have replaced $\eta(\mathbf{x}_i)$ by η_i and $\epsilon(\omega)$ is a normalization factor that depends only on the size of ω.

In the limit in which the volume of the cell can be regarded as small, we represent the free energy (5) by an integral over the volume of the system

$$F\{\eta\} = \int_\Omega d^3x\,[A\eta^2(\mathbf{x}) + B\eta^4(\mathbf{x})] \tag{7}$$

and the partition function by a functional integral over the space of functions $\eta(\mathbf{x})$ that satisfy appropriate boundary conditions and do not vary on a scale shorter than our graining

$$Z = \int \mathcal{D}\{\eta\}\, e^{-\beta F\{\eta\}} \tag{8}$$

where

$$\int \mathcal{D}\{\eta\} = \lim_{\omega \to 0} \int \prod_i \frac{d\eta_i}{\epsilon(\omega)}$$

The ensemble average of an arbitrary functional $\mathcal{F}\{\eta\}$ of $\eta(\mathbf{x})$ in this formalism will be defined by

$$\langle \mathcal{F}\{\eta\}\rangle = Z^{-1} \int \mathcal{D}\{\eta\}\, \mathcal{F}\{\eta\}\, e^{-\beta F\{\eta\}}$$

If we make the additional assumption that the mean value of η is the most probable one, then from Eqs. (7) and (8) we recover the results of Landau theory.[7] That is, we find that the most probable distribution of the field is uniform and the value $\bar{\eta}$ of the order parameter satisfies the equation

$$[A + 2B\bar{\eta}^2]\,\bar{\eta} = 0$$

On the other hand, if we do not replace the partition function (8) by its saddlepoint value and compute the order parameter correlation function taking the following ensemble average

$$\langle \eta(\mathbf{x})\,\eta(\mathbf{x}')\rangle = Z^{-1} \int \mathcal{D}\{\eta\}\, \eta(\mathbf{x})\,\eta(\mathbf{x}')\, e^{-\beta F\{\eta\}} \tag{9}$$

we see that there is no correlation for $\mathbf{x} \neq \mathbf{x}'$.

In fact, assuming that $\mathbf{x}$ is in the ith cell and $\mathbf{x}'$ in the i'th cell, Eq. (9) can be rewritten as

$$\langle \eta(\mathbf{x})\,\eta(\mathbf{x}')\rangle = \lim_{\omega \to 0} Z^{-1} \int_{-\infty}^{+\infty} \prod_j \frac{d\eta_j}{\epsilon(\omega)}\, \eta_i \eta_{i'} \exp\left[-\beta\omega \sum_j F(\eta_j)\right] \tag{10}$$

which vanishes for $i \neq i'$, $F(\eta_j)$ being an even function of its argument.

We arrive, therefore, at the conclusion that the free energy functional (7) is inadequate to describe a regime of the system where the cells are strongly interacting with each other as the previously mentioned divergence of the static susceptibility indicates.

In order to have a theory suited to describe the neighborhood of the transition, following Ferrell[1], we add to the local free energy density (4) a nonlocal contribution of the form

$$\eta(\mathbf{x}) \int d^s x'\, \lambda(|\mathbf{x} - \mathbf{x}'|)\, \eta(\mathbf{x}') \tag{11}$$

As it was remarked above, in the region of interest we expect long-wavelength variations to be dominant, hence we may expand $\eta(\mathbf{x}')$ in Taylor series and retain only the lower-order terms,

$$\eta(\mathbf{x}') = \eta(\mathbf{x}) + \mathbf{r} \cdot \nabla\eta(\mathbf{x}) + \tfrac{1}{2}\mathbf{rr} : \nabla\nabla\eta(\mathbf{x}) + \cdots, \qquad \mathbf{r} = (\mathbf{x}' - \mathbf{x})$$

Carrying out the integration, we see that from the invariance of the kernel $\lambda(|\mathbf{x} - \mathbf{x}'|)$ under rotation and reflection expression (11) reduces to $a\eta^2(\mathbf{x}) - A_0\eta(\mathbf{x})\, \nabla^2\eta(\mathbf{x})$, with

$$a = \int d^s r\, \lambda(|\mathbf{r}|) < 0, \qquad A_0 = -(1/2s) \int d^s r\, r^2 \lambda(|\mathbf{r}|) > 0$$

Adding this result to the free energy density in Eq. (10) we find the free energy functional

$$F\{\eta\} = \int d^s x\, [A_0(\nabla\eta)^2 + A\eta^2(\mathbf{x}) + B\eta^4(\mathbf{x}) - \mu(\mathbf{x})\,\eta(\mathbf{x})] \tag{12}$$

where the coefficient A has been corrected by a, and we have added a linear term in $\eta(\mathbf{x})$ to describe the more general case when there is coupling to an external field $\mu(\mathbf{x})$. The expansion of the nonlinear interaction term (11), however, is not essential to the development of the formalism presented in this paper. The partition function again is obtained by summing over all the possible distributions of the field.

$$Z = \int \mathscr{D}\{\eta\}\, e^{-\beta F\{\eta\}} \tag{13}$$

with $F\{\eta\}$ given by Eq. (12) and a similar modification holds for the definition of ensemble averages.

4. SPECIAL CASES

If we take the limit $B \to 0$, the functional integral equation (13) becomes Gaussian and various quantities can be evaluated exactly. For example, if we assume $T > T_c$ and $\mu = 0$, so that translational invariance holds, we find for the average order parameter

$$\langle\eta(\mathbf{x})\rangle_0 = Z^{-1}\int \mathscr{D}\{\eta\}\,\eta(\mathbf{x})\,e^{-\beta F_0\{\eta\}} = 0$$

where the subscript zero indicates that $B = 0$.

Furthermore, for the **k** Fourier component of the order parameter correlation function one finds

$$\int d^s r\, \langle\eta(\mathbf{x})\,\eta(\mathbf{x}')\rangle_0 \exp i\mathbf{k}\cdot\mathbf{r} = (2\beta[A_0k^2 + A])^{-1} \tag{14}$$

The $\mathbf{k} = 0$ component diverges as $A \to 0$ (T approaches T_c); this corresponds to the divergence of the susceptibility, thus the transition temperature coincides with T_c and the asymptotic behavior of the correlation function is of Ornstein–Zernike type.

For temperatures $T < T_c$ there is no stable value of the order parameter in the limit $B = 0$.

Another special case we want to consider is that the entire expression (12) for the free energy functional is retained but the integral (13) is replaced by the largest value of the integrand on the assumption that the mean value can be replaced by the most probable value. In other words, we assume that the fluctuations are very small.

As was stated in the introduction, this approximation leads to the classical results of the Landau–Ginzburg[26] theory.

Varying F in Eq. (12) with respect to η, it is found that the most probable value of the order parameter satisfies the Ginzburg–Landau equation

$$[2A + 4B\bar{\eta}^2(\mathbf{x}) - 2A_0\nabla^2]\,\bar{\eta}(\mathbf{x}) = \mu(\mathbf{x}) \tag{15}$$

If we now write $\mu \to \mu + \delta\mu$, correspondingly $\bar{\eta}$ changes by some $\delta\bar{\eta}$, and to first order we have

$$[2A + 12B\bar{\eta}^2(\mathbf{x}) - 2A_0\nabla^2]\,\delta\bar{\eta}(\mathbf{x}) = \delta\mu(\mathbf{x}) \tag{16}$$

On the other hand, the linear response of the average of $\eta(\mathbf{x})$ is given by $\delta\langle\eta(\mathbf{x})\rangle = \beta\int d^s x'\, q(\mathbf{x},\mathbf{x}')\,\delta\mu(\mathbf{x}')$, where

$$q(\mathbf{x},\mathbf{x}') = \langle[\eta(\mathbf{x}) - \langle\eta(\mathbf{x})\rangle][\eta(\mathbf{x}') - \langle\eta(\mathbf{x}')\rangle]\rangle \tag{17}$$

Equations (15) and (16) are used[6] to derive an expression for the correlation function q. This is done by identifying $\bar{\eta}(\mathbf{x})$ with $\langle\eta(\mathbf{x})\rangle$. The result is a correlation function of the Ornstein–Zernike type, yielding classical behavior for the susceptibility and the correlation length.

The identification depends, of course, on the absence of fluctuations.

But, as T_c is approached the susceptibility diverges and so the theory becomes inconsistent, leading to the Ginzburg criterion.[18] This limits the range of temperatures in which the approximation is applicable.

In summary, the remarks contained in this section, together with the arguments previously given for the necessity of the square-gradient term, show that in order to break away from a classical theory, both the correlating $(\nabla\eta)^2$ term and the nonlinear term $B\eta^4$ must be included in the free energy functional. Furthermore, averages must be computed from the partition function, rather than being substituted by most probable values. The rest of the paper will be concerned with the development of the formalism needed to achieve this aim.

5. DEFINITIONS AND DERIVATIVE RELATIONS

It is convenient to consider the more general form of the free energy functional (12)

$$F\{\eta\} = A(12)\,\eta(1)\,\eta(2) + B(1234)\,\eta(1)\,\eta(2)\,\eta(3)\,\eta(4) - \mu(1)\,\eta(1) \qquad (18)$$

where $1 = \mathbf{x}_1$, $2 = \mathbf{x}_2$, etc., integration over repeated indices is understood, and A and B are symmetric in their arguments.

The particular form (12) is recovered making the *ansatz*

$$A(12) = (A - A_0\nabla^2)\,\delta(1-2), \qquad B(1234) = B\,\delta(1-2)\,\delta(2-3)\,\delta(3-4) \qquad (19)$$

The thermodynamic average of an arbitrary functional $G\{\eta\}$ of the order parameter is defined by

$$\langle G\{\eta\}\rangle = Z^{-1}\int \mathscr{D}\{\eta\}\, G\{\eta\}\, e^{-\beta F\{\eta\}}$$

In particular, the n-point order parameter correlation function is the average of the functional $\eta(1)\,\eta(2)\cdots\eta(n)$,

$$g(12\cdots n) = \langle\eta(1)\,\eta(2)\cdots\eta(n)\rangle$$

so that in this notation the average local order parameter is the one-point correlation function $\langle\eta(1)\rangle = g(1)$.

From the relation between the thermodynamic free energy W and the partition function,

$$W = -\beta^{-1}\log Z \qquad (20)$$

it follows that the cumulants can be generated by functional differentiation of W with respect to μ:

$$q(12\cdots n) = (\beta^{-1})^{n-1}\left[\frac{\delta}{\delta\mu(n)}\frac{\delta}{\delta\mu(n-1)}\cdots\frac{\delta}{\delta\mu(1)}\right]W \tag{21}$$

where the derivatives are computed at the physical limit; that is, at the value of μ equal to the value of the external field.

In fact, from Eq. (21) it follows that the functions q are related to the correlation functions by

$$\begin{gathered} g(1) = q(1), \qquad g(12) = q(12) + q(1)\,q(2) \\ g(123) = q(123) + q(12)\,q(3) + q(13)\,q(2) + q(23)\,q(1) + q(1)\,q(2)\,q(3) \end{gathered} \tag{22}$$

etc.

Furthermore, the cumulants satisfy the derivative relation

$$\beta^{-1}[\delta/\delta\mu(n+1)]\,q(12\cdots n) = q(12\cdots n, n+1) \tag{23}$$

Similar relations satisfied by the correlation functions are

$$\begin{aligned} &\beta^{-1}[\delta/\delta\mu(n+1)]\,g(12\cdots n) = [g(12\cdots n+1) - g(12\cdots n)\,g(n+1)] \\ &\beta^{-1}[\delta/\delta A(n+1, n+2)]\,g(12\cdots n) \\ &\qquad = [g(12\cdots n+1, n+2) - g(12\cdots n)\,g(n+1, n+2)] \end{aligned} \tag{24}$$

For the later reference, we note that

$$\beta^{-1}\,\delta g(12)/\delta A(34) = [g(1234) - g(12)\,g(34)]$$

and expressing the correlation functions entering both sides of the equation in terms of the cumulants, we have

$$\begin{aligned} \beta^{-1}\,\delta q(12)/\delta A(34) = {} & [q(1234) + q(123)\,g(4) + q(124)\,g(3) \\ & + q(13)\,q(24) + q(14)\,q(23)] \end{aligned} \tag{25}$$

6. EQUATIONS FOR THE ORDER PARAMETER AND THE CORRELATION FUNCTION

The local average order parameter in absence of an external field is obtained by taking the limit

$$\lim_{\mu\to 0}\delta W/\delta\mu(1) = \lim_{\mu\to 0} g(1) \tag{26}$$

When translational invariance is assumed the r.h.s. becomes independent of position. The phase in which this average is nonzero is called the ordered phase and the other the disordered phase.[19] Let us first consider the latter case. An equation for the two-point correlation function can be immediately obtained from the identity[5]

$$\int \mathcal{D}\{\eta\}\,[\delta/\delta\eta(1)][\eta(2)\,e^{-\beta F\{\eta\}}] = 0 \tag{27}$$

In fact, carrying out the differentation under the integral, we obtain

$$\beta \langle \eta(2)\,\delta F\{\eta\}/\delta\eta(1)\rangle = \delta(1-2)$$

so that, computing explicitly the derivative and taking into account the symmetry of the coefficients in Eq. (18), the above equation becomes

$$2\beta A(1\bar{2})\,g(\bar{2}2) + 4\beta B(1\bar{2}34)\,g(\bar{2}342) = \delta(1-2)$$

or, in terms of the cumulants,

$$2\beta A(1\bar{2})\,q(\bar{2}2) + 4\beta B(1\bar{2}34)[3q(34)\,q(\bar{2}2) + q(\bar{2}342)] = \delta(1-2) \tag{28}$$

If we define the inverse function

$$q_0^{-1}(12) = 2\beta A(12) \tag{29}$$

and the analog of a "mass operator" $M(12)$ by

$$M(1\bar{2})\,q(\bar{2}2) = -4\beta B(1\bar{2}34)[3q(34)\,q(\bar{2}2) + q(\bar{2}342)] \tag{30}$$

Equation (28) can be cast in the form

$$[q_0^{-1}(1\bar{2}) - M(1\bar{2})]\,q(\bar{2}2) = \delta(1-2) \tag{31}$$

Equation (31) is similar to Dyson's equation for the Green's function in quantum field theory. We shall exploit this formal analogy to extend to this problem the techniques used in many-body theory to generate self-consistent approximation for the correlation function.

In the ordered phase the formalism is somewhat complicated by the occurrence of a nonvanishing value for the average order parameter.

We define a new field variable ξ describing the local fluctuations of the order parameter,

$$\xi(1) = \eta(1) - \nu(1) \tag{32}$$

[5] Wilson in the unpublished Ref. 8a has derived the Schwinger equation for q using the same approach only in the disordered phase. This work came to our attention only after the completion of the present work and we are grateful to Prof. Kenneth Wilson for bringing it to our attention. See also Ref. 27.

Then, in terms of ξ and g, the free energy functional (18) reads

$$F\{n\} = L\{g\} + G\{\xi, g\} \tag{33}$$

with

$$\begin{aligned}
L\{g\} &= A(12)\, g(1)\, g(2) + B(1234)\, g(1)\, g(2)\, g(3)\, g(4) - \mu(1)\, g(1) \\
G\{\xi, g\} &= A(12)[2g(1)\, \xi(2) + \xi(1)\, \xi(2)] \\
&\quad + B(1234)[4g(1)\, \xi(2)\, \xi(3)\, \xi(4) + 6g(1)\, g(2)\, \xi(3)\, \xi(4) \\
&\quad + 4g(1)\, g(2)\, g(3)\, \xi(4) + \xi(1)\, \xi(2)\, \xi(3)\, \xi(4)] - \mu(1)\, \xi(1)
\end{aligned} \tag{34}$$

As a consequence, for the partion function we have

$$Z = e^{-\beta L\{g\}}\, \mathscr{Z}\{g\} \tag{35}$$

with

$$\mathscr{Z}\{g\} = \int \mathscr{D}\{\xi\}\, e^{-\beta G\{\xi, g\}} \tag{36}$$

so that we the free energy becomes

$$W = L\{g\} - \beta^{-1} \log \mathscr{Z}\{g\} \tag{37}$$

The average of an arbitrary function $\mathscr{F}\{\xi\}$ will be defined by

$$\langle \mathscr{F}\{\xi\} \rangle = \mathscr{Z}^{-1}\{g\} \int \mathscr{D}\{\xi\}\, \mathscr{F}\{\xi\}\, e^{-\beta G\{\xi, g\}} \tag{38}$$

In particular, averages of products of the field variable ξ are referred to as subtracted correlation functions. We have

$$\begin{gathered}
\langle \xi(1) \rangle = 0, \qquad \langle \xi(1)\, \xi(2) \rangle = q(12), \qquad \langle \xi(1)\, \xi(2)\, \xi(3) \rangle = q(123) \\
\langle \xi(1)\, \xi(2)\, \xi(3)\, \xi(4) \rangle = q(1234) + q(12)\, q(34) + q(13)\, q(24) + q(14)\, q(23)
\end{gathered} \tag{39}$$

as follows from the definition (32) of the field variable ξ and the relations (22) between cumulants and correlation functions.

Thus, if we now consider the identity

$$\int \mathscr{D}\{\xi\}[\delta/\delta\xi(1)]\, e^{-\beta G\{\xi, g\}} = 0$$

and carry out the differentiation, we obtain $\langle \delta G\{\xi, g\}/\delta\xi(1) \rangle = 0$. That is,

$$2A(12)g(2) + 4B(1234)[3g(2)\, q(34) + g(2)\, g(3)\, g(4) + q(234)] - \mu(1) = 0 \tag{40}$$

where we have used Eqs. (34) and (39), and for generality we have kept a nonvanishing value for the external field. Defining the effective source function

$$K(1) = -4B(1234)[g(2)\,g(3)\,g(4) + 3g(2)\,q(34) + q(234)] \tag{41}$$

The above equation for the order parameter can be rewritten in the form

$$\beta^{-1}q_0^{-1}(12)\,g(2) = \mu(1) + K(1) \tag{42}$$

In principle, if we could solve exactly this functional equation for an arbitrary spatially varying external field, complete information on the equilibrium properties of the system would be obtained by generating correlation functions of higher order by functional differentiation of the solution for g with respect to μ. We see, however, from the definition (41) that K depends on g both explicitly and implicitly through the cumulants, and an exact solution is not possible.

In view of the necessity of turning to approximations, it is convenient to derive an equation also for the two-point cumulant. This allows us, on the one hand, to extend to the case where there is a condensed phase the techniques employed to generate systematically approximation schemes for "normal" systems, and on the other hand to regard the two-point cumulant as an independent variable in its own right, along with the order parameter as, for example, is the case in the so-called Φ-derivable approximation schemes.[20] Furthermore, for the kind of equilibrium properties of the system we are interested in, the order parameter and the two-point cumulant are the central objects in the theory. From the latter we may, in fact, easily derive the susceptibility in zero external field and the correlation length. Recalling that the susceptibility is given by the response of the average order parameter to a small uniform external field, we have

$$\chi = (1/\Omega)\int_\Omega d^s1\,[\delta g(1)/\delta\mu] \tag{43}$$

where, for a uniform variation of the external field,

$$\delta g(1)/\delta\mu = \beta\int_\Omega d^s2\,q(12) \tag{44}$$

Hence

$$\chi = (\beta/\Omega)\int_\Omega d^s1\,d^s2\,q(12) \tag{45}$$

Since we consider uniform variations of μ, translational invariance holds, so that

$$\chi = \beta\int_\Omega d^s(1-2)\,q(1-2) = \beta q(k=0) \tag{46}$$

where

$$q(k) = \int_\Omega d^s(1-2)\, e^{ik(1-2)} q(1-2) \tag{47}$$

For the correlation length we have

$$\xi^2 = \frac{\int_\Omega d^s(1-2)\,(1-2)^2\, q(1-2)}{\int_\Omega d^s(1-2)\, q(1-2)} = -\frac{1}{\chi}\frac{\partial^2 q(k)}{\partial k^2}\Big|_{k=0} \tag{48}$$

To derive the equation satisfied by the two-point cummulant, we consider the identity

$$\mathscr{Z}^{-1}\{g\}\int \mathscr{D}\{\xi\}\,[\delta/\delta\xi(1)][\xi(2)\, e^{-\beta G\{\xi,g\}}] = 0 \tag{49}$$

Carrying out the derivation, we obtain

$$\begin{aligned}2\beta A(1\bar{2})\langle\xi(\bar{2})\,\xi(2)\rangle &+ 4\beta B(1\bar{2}34)[3g(\bar{2})\langle\xi(3)\,\xi(4)\,\xi(2)\rangle \\ &+ 3g(3)\,g(4)\langle\xi(\bar{2})\,\xi(2)\rangle + \langle\xi(\bar{2})\,\xi(3)\,\xi(4)\,\xi(2)\rangle] = \delta(1-2)\end{aligned}$$

where we have used Eq. (34) and the first of Eqs. (39). Comparing this with the rest of Eqs. (39), we obtain

$$\begin{aligned}2\beta A(1\bar{2})\,q(\bar{2}2) &+ 4\beta B(1\bar{2}34)[3g(3)\,g(4)\,q(\bar{2}2) + 3q(34)\,q(\bar{2}2) \\ &+ 3g(\bar{2})\,q(342) + q(\bar{2}342)] = \delta(1-2)\end{aligned} \tag{50}$$

We may now define the analog of the "mass operator" by

$$\begin{aligned}M(1\bar{2})\,q(\bar{2}2) = &-4\beta B(1\bar{2}34)[3g(3)\,g(4)\,q(\bar{2}2) + 3q(34)\,q(\bar{2}2) \\ &+ 3g(\bar{2})\,q(342) + q(\bar{2}342)]\end{aligned} \tag{51}$$

so that, making the appropriate insertion on the l.h.s., Eq. (50) takes the same form as Eq. (31), i.e.,

$$[q_0^{-1}(1\bar{2}) - M(1\bar{2})]\,q(\bar{2}2) = \delta(1-2) \tag{52}$$

We shall now make some considerations that depend only on the form of Eq. (52).

7. TRANSITION TEMPERATURE AND STRONG COUPLING

In Section 3 we introduced the parameters of the model and among these appeared T_c. This temperature was included in order to facilitate the comparison with previous calculations, mainly Landau's.[7] However, when one treats the statistical mechanics of the model as expressed in Eqs. (1)

and (2), T_r loses any particular meaning. Since the model is supposed to describe a system near a transition, we have to define a transition temperature within the theory.

A natural definition results immediately from the relation between the susceptibility and the cumulant q, Eq. (46). At the transition temperature the susceptibility diverges and hence we can define T_r as the temperature at which

$$q^{-1}(k = 0, T_r) = 0 \tag{53}$$

This definition applies both in the ordered and disordered phases.

We mention in passing another possibility for defining T_r, namely the temperature at which g vanishes. In other words, we expect that at low temperatures Eq. (42) for the order parameter will possess nonvanishing solutions in the uniform system and with external field $\mu = 0$. As the temperature is increased these solutions tend to zero. T_r can be defined as the temperature at the which they vanish. The matching of the different definitions of T_r is no minor burden on an approximation scheme.

Considering the Fourier transforms of q and q_0, which are defined in the uniform case by

$$q(12) = (1/\Omega) \sum_k e^{ik(1-2)} q(k) \tag{54}$$

$$q_0(12) = (1/\Omega) \sum_k e^{ik(1-2)} q_0(k) \tag{55}$$

and also

$$M(12) = (1/\Omega) \sum_k e^{ik(1-2)} M(k) \tag{56}$$

Eq. (52) can be rewritten as

$$q(k) = [q_0^{-1}(k) - M(k)]^{-1} = [2\beta A(k) - M(k)]^{-1} \tag{57}$$

where use was made of Eq. (29). All the functions appearing in (57) depend, of course, on T also. The equation for T_r, (53), reads

$$2\beta_r A(0, T_r) - M(0, T_r) = 0 \tag{58}$$

From (57) and (58) we have

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

which we consider in two limits:

(a) $T = T_r$, $k \to 0$. Here

$$q^{-1}(k, T_r) = 2\beta_r [A(k, T_r) - A(0, T_r)] - [M(k, T_r) - M(0, T_r)] \tag{59}$$

From the arguments leading to (12), one expects

$$A(k, T_r) - A(0, T_r) \underset{k \to 0}{\sim} A_0 k^2 \tag{60}$$

At T_r the inverse correlation function should behave as $k^{2-\eta}$, $\eta > 0$.[6] If indeed $\eta > 0$, then the critical behavior of $q^{-1}(k)$ has to come from the second term in Eq. (59), namely from

$$M(k, T_r) - M(0, T_r) \underset{k \to 0}{\sim} k^{2-\eta}$$

which will dominate the first term as $k \to 0$.

The situation is more interesting in the next case.

(b) $k = 0$, $T \to T_r$. Here

$$\begin{aligned} q^{-1}(0, T) &= 2\beta A(0, T) - 2\beta_r A(0, T_r) - [M(0, T) - M(0, T_r)] \\ &= 2\beta[A(0, T) - A(0, T_r)] + 2(\beta - \beta_r) A(0, T_r) \\ &\quad - [M(0, T) - (0, T_r)] \end{aligned} \tag{61}$$

If $A(12)$ is taken from Eq. (19) with

$$A(0, T) = \alpha(T - T_r) \tag{62}$$

as in the discussion leading to Eq. (4), then

$$A(0, T) - A(0, T_r) = \alpha(T - T_r) \tag{63}$$

If A were independent of T, the first term in Eq. (61) would vanish. The second term on the r.h.s. of Eq. (61) is clea ly linear in $T - T_r$. But as we know[6]

$$q^{-1}(0, T) = \beta\chi^{-1}(T) \underset{T \to T_r}{\sim} (T - T_r)^{\gamma} \tag{64}$$

with $\gamma > 1$. Thus the linear term in $T - T_r$ has to be *exactly* canceled by the third term on the r.h.s. of (61). If the third term in (61) were merely to produce $(T - T_r)^{\gamma}$, that would not suffice, since near T_r the linear term would dominate for $\gamma > 1$.

From Eq. (51) it is evident that as $B \to 0$, $M \to 0$. The linear term in $T - T_r$ is independent of B. The conclusion is that as $T \to T_r$, M cannot have a weak coupling limit. Whatever the size of B, there is always a value $T - T_r$ such that for all T satisfying

$$|T - T_r| < B^{\rho}, \qquad \rho > 0$$

$M(0, T) - M(0, T_r)$ will have a leading term in $T - T_r$ whose coefficient is independent of B.

This is a result beyond the power of any finite perturbation expansion in B.

8. RENORMALIZED EQUATIONS FOR K AND M

We notice that if we let the average of the order parameter vanish, the functional M defined in Eq. (51) coincides with the corresponding functional defined in Eq. (30) and the solutions of Eq. (52) tend to the solutions of Eq. (31).

It is therefore convenient to develop the formalism in the ordered phase; the description of the disordered phase will then be contained as a particular case obtained by setting to zero the value of the external field and of the average order prameter. Equations (42) and (52) are the first two of an infinite chain of equations relating cumulants of higher and higher order. We can formally close the set of equations by eliminating three-point and four-point cumulants from the expressions for K and M, at the expense of introducing a functional integrodifferential equation for M.

Such a step does not represent any progres stoward the exact solution of the problem; however, it has the advantage that approximation schemes can be derived systematically by iteration of the equation for M.[9,21]

The elimination of three- and four-point cumulants is carried out using the derivative relations (23), (25), and Dyson's equation, with the result (see Appendix A)

$$\begin{aligned} M(12) = {} & -4\beta B(1234)[3g(3)\,g(4) + 3q(34)] \\ & + 4B(1\bar{2}34)\{g(\bar{2})\,q(3\bar{3})[\delta M(\bar{3}2)/\delta\mu(4)] + q(\bar{2}3)[\delta M(\bar{3}2)/\delta A(34)]\} \end{aligned} \tag{65}$$

which in the disordered phase reduces to

$$M(12) = -12\beta B(1234)\,q(34) + 4B(1\bar{2}34)\,q(\bar{2}\bar{3})[\delta M(\bar{3}2)/\delta A(34)] \tag{66}$$

We must now express the derivatives with respect to μ and A in terms of derivatives with respect to the natural variables g and q. The method is closely similar to the renormalization procedure for the source function and the mass operator in Ref. 11.

M depends on μ and A only through g and q. That this is so can be seen by generating the skeleton diagrams for M by iteration of Eq. (65) and observing that they contain only the bare interaction B, g lines, and q lines.

Thus, we may write

$$\begin{aligned} \frac{\delta M(12)}{\delta\mu(3)} &= \left[\frac{\delta M(12)}{\delta g(\bar{3})}\right]_q \frac{\delta g(\bar{3})}{\delta\mu(3)} + \left[\frac{\delta M(12)}{\delta q(\bar{3}4)}\right]_g \frac{\delta q(\bar{3}4)}{\delta\mu(3)} \\ &= \beta\left[\frac{\delta M(12)}{\delta g(\bar{3})}\right]_q q(\bar{3}3) + \left[\frac{\delta M(12)}{\delta q(\bar{3}4)}\right]_g q(\bar{3}5)\,\frac{\delta M(54)}{\delta\mu(3)}\,q(\bar{4}4) \end{aligned}$$

where Eq. (A.2) of Appendix A was used.

Defining

$$\Lambda^{-1}(1234) = \delta(1-3)\,\delta(2-4) - [\delta M(12)/\delta q(\bar3\bar4)]_g\, q(\bar3 3)\, q(\bar4 4) \tag{67}$$

we obtain

$$\delta M(12)/\delta\mu(3) = \beta\Lambda(12\bar1\bar2)[\delta M(\bar1\bar2)/\delta g(\bar3)]_q\, q(\bar3 3) \tag{68}$$

Similarly, from

$$\frac{\delta M(12)}{\delta\Lambda(34)} = \left[\frac{\delta M(12)}{\delta g(\bar3)}\right]_q \frac{\delta g(\bar3)}{\delta\Lambda(34)} + \left[\frac{\delta M(12)}{\delta q(\bar3\bar4)}\right]_g \frac{\delta q(\bar3\bar4)}{\delta\Lambda(34)}$$

we obtain (see Appendix B)

$$\begin{aligned}\frac{\delta M(12)}{\delta\Lambda(34)} = {} & \beta\Lambda(12\bar1\bar2)\left[\frac{\delta M(\bar1\bar2)}{\delta g(\bar3)}\right]_q [g(3)\, q(\bar3 4) + g(4)\, q(\bar3 3)]\\ & + \beta\Lambda(12\bar1\bar2)\left[\frac{\delta M(\bar1\bar2)}{\delta q(\bar3\bar4)}\right]_g [q(\bar3 3)\, q(\bar4 4) + q(\bar3 4)\, q(\bar4 3)]\\ & + \beta\Lambda(12\bar1\bar2)\left[\frac{\delta M(\bar1\bar2)}{\delta g(\bar3)}\right]_q q(\bar3 5)\, \Lambda(56\bar5\bar6)\left[\frac{\delta M(\bar5\bar6)}{\delta g(\bar7)}\right]_q q(\bar7 4)\, q(\bar6 3)\end{aligned} \tag{69}$$

Inserting Eqs. (68) and (69) in Eq. (65), the announced integrodifferential equation for M is obtained; however, in order to have the equations in a form more suitable for generating approximation schemes, we make a few additional formal manipulations.

Recognizing that the derivative of M with respect to q gives the irreducible vertex part[22]

$$\Xi(1234) = [\delta M(12)/\delta q(34)]_g \tag{70}$$

we proceed to show that the four-point vertex function

$$\Gamma(1234) = \Lambda(12\bar1\bar2)[\delta M(\bar1\bar2)/\delta q(34)]_g$$

satisfies the Bethe–Salpeter equation. In fact, the definition

$$\Lambda^{-1}(1234) = \delta(1-3)\,\delta(2-4) - \Xi(12\bar3\bar4)\, q(\bar3 3)\, q(\bar4 4)$$

can be used to obtain the formal expansion

$$\begin{aligned}\Lambda(1234) = {} & \delta(1-3)\,\delta(2-4) + \Xi(12\bar3\bar4)\, q(\bar3 3)\, q(\bar4 4)\\ & + \Xi(12\bar3\bar4)\, q(\bar3 5)\, q(\bar4 6)\, \Xi(56\bar5\bar6)\, q(\bar5 3)\, q(\bar6 4) + \cdots\end{aligned}$$

Thus, for Γ we have

$$\begin{aligned}\Gamma(1234) = {} & \Xi(1234) + \Xi(12\bar1\bar2)\, q(\bar1 5)\, q(\bar2 6)[\delta(5-\bar3)\,\delta(6-\bar4)\\ & + \Xi(5678)\, q(7\bar3)\, q(8\bar4) + \cdots]\, \Xi(\bar3\bar4 34)\end{aligned}$$

and resumming the series, we find that Γ satisfies

$$\Gamma(1234) = \Xi(1234) + \Xi(12\bar{1}\bar{2})\, q(\bar{1}5)\, q(\bar{2}6)\, \Gamma(5634) \tag{71}$$

which is the Bethe–Salpeter equation.

Similarly, we may define the three-point irreducible vertex part

$$X(123) = [\delta M(12)/\delta g(3)]_q \tag{72}$$

and show that the three-point vertex function

$$P(123) = \Delta(12\bar{1}\bar{2})[\delta M(\bar{1}\bar{2})/\delta g(3)]_q \tag{73}$$

is related to Γ by the equation (see Appendix C)

$$P(123) = X(123) + \Gamma(12\bar{1}\bar{2})\, q(\bar{1}5)\, q(\bar{2}6)\, X(563) \tag{74}$$

Rewriting Eqs. (68) and (69) in terms of the vertex functions and inserting the result in Eqs. (A.4) and (A.5) of Appendix A, we obtain

$$K(1) = 4B(1234)[g(2)\, g(3)\, g(4) + 3g(2)\, q(34) + q(2\bar{2})\, q(3\bar{3})\, P(\bar{2}\bar{3}6)\, q(64)] \tag{75}$$

$$\begin{aligned} M(12) = & -4\beta B(1234)[3g(3)\, g(4) + 3q(34)] \\ & - 4\beta B(1\bar{2}34)\, g(\bar{2})\, q(3\bar{3})\, P(\bar{3}26)\, q(64) \\ & - 4\beta B(1\bar{2}34)\, q(\bar{2}\bar{3})\, P(\bar{3}26)[g(3)\, q(64) + g(4)\, q(63)] \\ & - 4\beta B(1\bar{2}34)\, q(\bar{2}\bar{3})\, \Gamma(\bar{3}267)[q(63)\, q(74) + q(64)\, q(73)] \\ & \quad 4\beta B(1\bar{2}34)\, q(\bar{2}\bar{3})\, P(\bar{3}26)\, q(67)\, P(789)\, q(94)\, q(93) \end{aligned} \tag{76}$$

Equations (42), (52), (75) (76), (71), and (74) together with the definitions (70) and (72) of Ξ and X provide the desired of equations.

In the disordered phase, g, K, X, and P vanish identically and the set of equations reduces to Dyson's equation, with M given by

$$\begin{aligned} M(12) = & -12\beta B(1234)\, q(34) \\ & - 4\beta B(1\bar{2}34)\, q(\bar{2}\bar{3})\, \Gamma(\bar{3}267)[q(63)\, q(74) + q(64)\, q(73)] \end{aligned} \tag{77}$$

and the Bethe–Salpeter equation for Γ, Eq. (71), with Ξ defined by

$$\Xi(1234) = \delta M(12)/\delta q(34) \tag{78}$$

9. APPROXIMATION SCHEMES

If we assume that B is a small quantity, we may think of treating the nonlinear interaction by means of ordinary perturbation theory.

In the disordered phase this amounts to computing the noninteracting correlation function q_0 in the soluble model $B = 0$, thereafter generating expansions for M in terms of B and q_0 by iteration of Eq. (66).[21]

However, this method cannot be extended to the region below the transition since, as has been already pointed out, for $B = 0$ there is no stable order parameter and the noninteracting correlation function is ill-defined.

Furthermore, the absence of a weak coupling limit, which we have discussed in Section 7 and which was pointed out as well by Ferrell,[11] clearly shows that even in the disordered phase ordinary perturbation theory is insufficient to describe the behavior of the system at the transition. It is therefore necessary to consider self-consistent approximation of infinite order in B. The formal results of the previous section provide the mechanism for generating such approximations in a systematic way.

The most simple approximation schemes are obtained taking K and M to some order in g and q and solving self-consistently the couple of equations (42) and (52). However, care must be exercised in matching the approximation for M with the approximation for K. In this one is guided by relations satisfied by the exact M and K. For example, differentiating Eq. (42) with respect to μ, we obtain the equation

$$\beta^{-1} q_0^{-1}(1\bar{2})\, \delta g(\bar{2})/\delta\mu(2) = \delta(1-2) + [\delta K(1)/\delta\mu(2)] \qquad (79)$$

Next, if K is regarded as a functional of g only, we may write

$$\delta K(1)/\delta\mu(2) = [\delta K(1)/\delta g(\bar{2})]\, \delta g(\bar{2})/\delta\mu(2) \qquad (80)$$

and inserting this in Eq. (79), it follows that

$$\{q_0^{-1}(1\bar{2}) - \beta[\delta K(1)/\delta g(\bar{2})]\}\, \beta^{-1}\, \delta g(\bar{2})/\delta\mu(2) = \delta(1-2) \qquad (81)$$

Recalling the derivative relation (23) and comparing with Eq. (52), we see therefore that in the exact theory M and K are related by

$$M(12) = \beta\, \delta K(1)/\delta g(2) \qquad (82)$$

In the theory of interacting bosons approximations that preserve the above relation between M and K do satisfy the Hugenholtz-Pines theorem and are therefore referred to as "gapless" approximations.[20],[6]

However, if the approximation is such that Eq. (82) is not satisfied, then Eqs. (81) and (52) it follows that $q(12) \neq \beta^{-1}\, \delta g(1)/\delta\mu(2)$. That is, within

[6] This analogy should not be taken too literally. In fact, for the boson system the Hugenholtz–Pines theorem is a consequence of the gauge invariance of the theory, which does not hold in the present case.

the considered approximation the correlation function cannot be related to the response of the order parameter to an external disturbance. To put it differently, only in the case of "gapless" approximations may we derive unambiguously the static susceptibility from $q(k \to 0)$. We represent Eq. (75) pictorially as follows:

K = 

where the completely symmetric interaction is denoted by a dot, the curly line represents the order parameter g, the full line represents the two-point cumulant q, and the triangle represents the three-point vertex function P. We see that the simplest approximation to K is given by the term

 $-4B(1234)g(2)g(3)g(4)$ (83)

Hence, the corresponding "gapless" approximation is generated by taking for M the diagram obtained by differentiating (83) with respect to g:

 $-12B(1234)g(3)q(4)$ (84)

Diagrams of this type for M and K correspond to the Bogoliubov approximation for liquid helium.[20] Inserting expressions (83) and (84) in Eqs. (42) and (52) and specializing to the translational invariant case of a uniform external field, the following equations are obtained after making the *ansatz* (19) for A and B:

$$2[A + 2Bg^2]g = \mu, \qquad 2\beta[A - A_0\nabla^2 + 6Bg^2]\, q(1-2) = \delta(1-2) \quad (85)$$

The first of the above equations is the equation for the order parameter obtained in the Landau theory,[7] while the second one is the equation for the correlation function obtained by Kadanoff *et al.*[6]

Therefore, it appears that the classical theory corresponds to the first and most simple approximation in the hierachy generated by taking into account successive diagrams for K.

We just mention here, and shall reconsider the subject more extensively in the next section, that alternatively to the "gapless" scheme there exists the so-called Φ-derivable approximation scheme. In Φ-derivable approximations Eq. (82), satisfied by M and K in the exact theory, need no longer be satisfied by the approximate M and K.

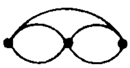
Such a distinction, however, does not exist in the disordered phase where in zero field K is identically zero. In this case one has only to produce approximate expressions for M as a functional of q and solve self-consistently Eq. (31). Considering Eq. (66), the lowest-order contribution to M is given by the Hartree term

$$-12\beta B(123\bar{4})q(\bar{3}\bar{4}) \tag{86}$$

Iterating, one finds to second order

$$6(4\beta)^2 B(1\bar{3}\bar{4}\bar{5})q(\bar{3}\bar{\bar{3}})B(\bar{\bar{3}}2\bar{\bar{4}}\bar{\bar{5}})q(\bar{4}\bar{\bar{4}})q(\bar{5}\bar{\bar{5}})$$

and to third order



$$54(4\beta)^3 B(1\bar{3}\bar{4}\bar{5})q(\bar{3}\bar{\bar{3}})B(\bar{\bar{3}}\bar{\bar{4}}\bar{6}\bar{7})q(\bar{4}\bar{\bar{4}})q(\bar{6}\bar{\bar{6}})$$
$$\times B(\bar{\bar{6}}2\bar{\bar{7}}\bar{\bar{5}})q(\bar{7}\bar{\bar{7}})q(\bar{5}\bar{\bar{5}})$$

Inserting expression (86) for M in Eq. (31) and making again the *ansatz* (19), for the translational invariant system we find the following equation for the correlation function:

$$2\beta[A - A_0\nabla^2 + 6Bq(1 - \bar{2})]\,\delta(1 - \bar{2})\,q(\bar{2} - 2) = \delta(1 - 2)$$

In a forthcoming paper we shall consider the self-consistent solution of the above equation, which exhibits a "nonclassical" asymptotic behavior for the susceptibility, and the problem of extending the approximation below the transition.

As was already mentioned, the lack of weak coupling limit compels one to consider self-consistent approximations of infinite order in B. To go beyond the simple schemes of the type mentioned above, one must make full use of the closed set of equations obtained in the previous section.

The general scheme can be summarized so: From an initial approximate expression for M as a functional of the unknown g and q the irreducible vertex parts Ξ and X are computed by functional differentiation. Ξ is used in Eq. (71) to solve for Γ, and P is calculated form Eq. (74). In turn Γ and P are inserted in the equations for K and M, (75) and (76), respectively, which must be solved self-consistently together with the equations for g and q.

In its simplest version this program gives the shielded potential approximation for the correlation function. Limiting ourselves to the disordered phase and taking as the initial approximation for M the Hartree term

from Eq. (78), Ξ reduces to the bare interaction •. Inserting this result in Eq. (71), Γ is obtained as the sum of all bubble diagrams

$\Gamma =$ 

Substituting in turn into Eq. (77) and iterating, we find that M is given by the sum of all diagrams obtained by removing one q-line from the bubble ring diagrams:

$M =$ 

Going one step further and deriving from the above expression for M the irreducible vertex part Ξ ,we obtain an equation for Γ formally similar to the one considered by Riedel.[23]

10. FREE ENERGY

As we have seen previously, quantities like the susceptibility and the correlation length can be readily obtained once the order parameter correlation function is known.

However, another quantity of interest is the specific heat and this cannot be obtained just from the knowledge of the correlation function. In order to obtain the general thermodynamic properties of the system associated with a given approximation to the correlation function one needs an expression for the free energy as a functional of g and q

One can show that a Luttinger–Ward[10,11] type of free energy expression can be obtained, namely

$$\beta W = \beta\mu(1)\,g(1) - \beta A(12)[g(1)\,g(2) - q(12)] + \tfrac{1}{2}\log q(1,1) + \tfrac{1}{2}\beta\Phi\{g,q\} \tag{87}$$

where the notation $\log q(1,1)$ represents the trace of the matrix $\log q(1,2)$. If the system is translationally invariant, then the matrix is diagonal in the momentum representation and $\log q(1,1)$ can be computed summing over the Fourier components $\sum_p \log q(p)$.

The functional $\Phi\{g,q\}$ has the following properties:

$$[\delta\Phi/\delta g(1)]_q = 2K(1), \qquad [\delta\Phi/\delta q(1,2)]_g = \beta^{-1}M(1,2) \tag{88}$$

In order to show that Eq. (87) indeed gives an expression for the free energy, one computes the derivatives of the r.h.s. with respect to the parameters A, B, β, obtaining (Appendix D)

$$\delta(-\beta W)/\delta A(12) = \beta[g(1)\,g(2) + q(12)] \tag{89}$$

$$\begin{aligned}\partial(-\beta W)/\partial B = \beta[&g^4(1) + 6g^2(1)\,q(11) + 3q^2(11)\\ &+ 4g(1)\,q(111) + q(1111)]\end{aligned} \tag{90}$$

$$\begin{aligned}\partial(-\beta W)/\partial\beta = &[\mu(1) - A(12)\,g(2) + \tfrac{1}{4}K(1)]\,g(1)\\ &+ [\tfrac{1}{2}\beta^{-1}M(12) - A(12)]\,q(12)\end{aligned} \tag{91}$$

In Eq. (90) all arguments of the cumulants are taken at the same point and an integration over the volume of the system is understood. The derivative with respect to B, for simplicity, has been computed in the case of a point interaction, corresponding to the *ansatz* (19).

In the exact case these derivatives are equal to the corresponding derivatives of $\log Z$ (Appendix D), where Z is the partition function given in Eq. (35).

Furthermore, differentiating $(-\beta W)$ with respect to g and q, keeping the parameters constant, it follows that

$$[\delta(-\beta W)/\delta g(1)]_q = \beta\mu(1) + \beta K(1) - q_0^{-1}(12)\,g(2)$$

$$[\delta(-\beta W)/\delta q(12)]_g = \tfrac{1}{2}[q_0^{-1}(12) - M(12) - q^{-1}(12)]$$

Therefore, comparing with Eqs. (42) and (52), we find

$$[\delta(-\beta W)/\delta g(1)]_q = [\delta(-\beta W)/\delta q(12)]_g = 0 \tag{92}$$

That is, the expression for the free energy given in Eq. (87) has the property that it is stationary for changes of g and q about their physical values, when the parameters are kept fixed.

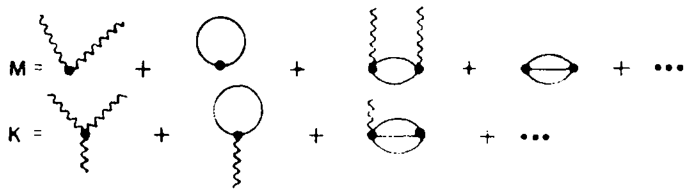
Note that the variational property, as well as the functional form of the derivatives given in Eqs. (89)–(91) depends only on the following conditions: (a) M and K are obtained from a functional Φ according to Eq. (88); (b) g and q are solved self-consistently. Namely, they satisfy Eqs. (42) and (52).

Therefore, for any Φ-derivable approximation[10,20] namely any approximation that satisfies conditions (a) and (b) above, the free energy is stationary for variations of g and q about their physical values. In addition, its derivatives with respect to the parameters have the same functional form as the derivatives of the exact free energy.

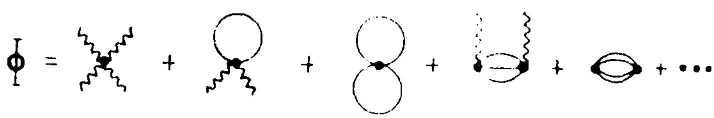
The Φ-derivability of the approximation guarantees the unambiguous determination of the free energy. Furthermore, the variational property can serve as an important tool for obtaining nonperturbative approximations for g and q.

In general a Φ-derivable approximation is not at the same time a "gapless" approximation.

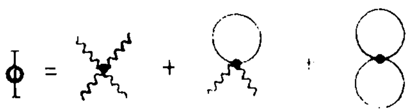
To illustrate this point, we construct the diagrams for M and K by iteration of Eq. (65) and Eq. (A.4) of Appendix A:



Then, with the help of Eq. (88), we can infer the form of the diagrams entering the expansion of Φ:

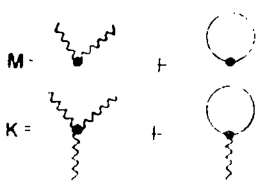


If we take, for example, the following approximation for Φ:



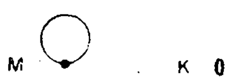
(93)

then, according to Eq. (88), it follows that



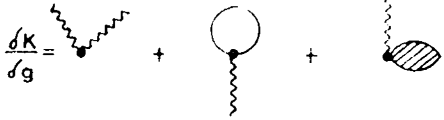
(94)

In the disordered phase these diagrams reduce to



which is just the Hartree approximation mentioned in Section 9.

In the ordered phase the expressions (94) for M and K generate a couple of equations for g and q of the type encountered in the Girardeau–Arnowitt approximation for liquid helium.[20–25] Such an approximation, though, is not "gapless." In fact, when K is regarded as a functional of g only, we have



(95)

where

denotes the sum of the terms obtained taking the derivative with respect to g inside q in the Hartree term. Comparing with the first Eq. (94), we see that Eq. (82) is not satisfied.

APPENDIX A. DERIVATION OF EQ. (65)

From the identity

$$\delta q(12)/\delta\mu(3) = -q(1\bar{2})[\delta q^{-1}(\bar{2}\bar{3})/\delta\mu(3)]\, q(\bar{3}2) \tag{A.1}$$

and Eq. (52), we obtain

$$\frac{\delta q(12)}{\delta\mu(3)} = q(1\bar{2})\,\frac{\delta M(\bar{2}\bar{3})}{\delta\mu(3)}\, q(\bar{3}2) \tag{A.2}$$

$$(-\beta^{-1})\,\frac{\delta q(12)}{\delta A(34)} = q(13)\,q(42) + q(14)\,q(32) - \beta^{-1}q(1\bar{2})\,\frac{\delta M(\bar{2}\bar{3})}{\delta A(34)}\, q(\bar{3}2) \tag{A.3}$$

where to derive Eq. (A.3) we have used the symmetry of A: $2A(12) = A(12) + A(21)$.

Employing the derivative relation (23), the l.h.s. of Eq. (A.2) can be expressed in terms of the three point cumulant and inserting in Eq. (41) we obtain

$$K(1) = -4B(1234)\left[g(2)\,g(3)\,g(4) + 3g(2)\,q(34) - \beta^{-1}q(2\bar{2})\,\frac{\delta M(\bar{2}\bar{3})}{\delta\mu(4)}\, q(\bar{3}3)\right] \tag{A.4}$$

Next we observe that Eq. (51), from the symmetry of the parameter B, can be rewritten as

$$\begin{aligned} M(1\bar{2})\,q(\bar{2}2) = -4\beta B(1\bar{2}34)[&3g(3)\,g(4)\,q(\bar{2}2) + q(34)\,q(\bar{2}2) + g(\bar{2})\,q(342) \\ &+ q(\bar{2}234) + q(\bar{2}23)\,g(4) + q(\bar{2}24)\,g(3) + q(\bar{2}3)\,q(24) \\ &+ q(\bar{2}4)\,q(23)] \end{aligned}$$

Hence, comparing with Eq. (18),

$$\begin{aligned} M(1\bar{2})\,q(\bar{2}2) = -4\beta B(1\bar{2}34)\{&3g(3)\,g(4)\,q(\bar{2}2) + q(34)\,q(\bar{2}2) + g(\bar{2})\,q(342) \\ &+ (-\beta^{-1})[\delta q(\bar{2}2)/\delta A(34)]\} \end{aligned}$$

inserting Eqs. (A.2) and (A.3) in the r.h.s. and multiplying by q^{-1}, we finally obtain Eq. (65):

$$
\begin{aligned}
M(12) = {} & 4\beta B(1234)[3g(3)\,g(4) + 3q(34)] \\
& - 4B(1\bar{2}34)\{g(2)\,q(3\bar{3})[\delta M(\bar{3}2)/\delta\mu(4)] - q(\bar{2}\bar{3})[\delta M(\bar{3}2/\delta A(34)]\}
\end{aligned}
\tag{A.5}
$$

APPENDIX B. DERIVATION OF EQ. (69)

From the second derivative relation (17) and Eq. (A.2), we have

$$
\begin{aligned}
\delta g(\bar{3})/\delta A(34) &= -\beta[g(\bar{3}34) - g(3)\,g(34)] \\
&= -\beta[q(\bar{3}34) + g(3)\,q(\bar{3}3) + g(4)\,q(\bar{3}3)] \\
&\quad -\beta[g(3)\,q(\bar{3}4) + g(4)\,q(\bar{3}3)] - q(\bar{3}5)][\delta M(56)/\delta\mu(4)]\,q(63)
\end{aligned}
$$

while from Eq. (A.3)

$$
\frac{\delta q(\bar{3}\bar{4})}{\delta A(34)} = -\beta[q(\bar{3}3)\,q(\bar{4}4) + q(\bar{3}4)\,q(\bar{4}3)] + q(\bar{3}5)\,\frac{\delta M(56)}{\delta A(34)}\,q(6\bar{4})
$$

Hence, substituting in

$$
\frac{\delta M(12)}{\delta A(34)} = \left[\frac{\delta M(12)}{\delta g(\bar{3})}\right]_q \frac{\delta g(\bar{3})}{\delta A(34)} + \left[\frac{\delta M(12)}{\delta q(\bar{3}\bar{4})}\right]_g \frac{\delta q(\bar{3}\bar{4})}{\delta A(34)}
$$

we obtain

$$
\begin{aligned}
\frac{\delta M(12)}{\delta A(34)} = {} & -\beta\left[\frac{\delta M(12)}{\delta g(\bar{3})}\right]_q [g(3)\,q(\bar{3}4) + g(4)\,q(\bar{3}3)] \\
& - \left[\frac{\delta M(12)}{\delta g(\bar{3})}\right]_q q(\bar{3}5)\,\frac{\delta M(56)}{\delta\mu(4)}\,q(63) \\
& - \beta\left[\frac{\delta M(12)}{\delta q(\bar{3}\bar{4})}\right]_g [q(\bar{3}3)\,q(\bar{4}4) + q(\bar{3}4)\,q(\bar{4}3)] \\
& + \left[\frac{\delta M(12)}{\delta q(\bar{3}\bar{4})}\right]_g q(\bar{3}5)\,q(\bar{4}6)\,\frac{\delta M(56)}{\delta A(34)}
\end{aligned}
$$

This can be rewritten as

$$
\begin{aligned}
\frac{\delta M(12)}{\delta A(34)} - \left[\frac{\delta M(12)}{\delta q(\bar{3}\bar{4})}\right]_g q(\bar{3}5)\,q(\bar{4}6)\,\frac{\delta M(56)}{\delta A(34)} \\
= -\beta\left[\frac{\delta M(12)}{\delta g(\bar{3})}\right]_q [g(3)\,q(\bar{3}4) + g(4)\,q(\bar{3}3)] \\
-\beta\left[\frac{\delta M(12)}{\delta q(\bar{3}\bar{4})}\right]_g [q(\bar{3}3)\,q(\bar{4}4) + q(\bar{3}4)\,q(\bar{4}3)] \\
- \left[\frac{\delta M(12)}{\delta g(\bar{3})}\right]_q q(\bar{3}5)\,\frac{\delta M(56)}{\delta\mu(4)}\,q(63)
\end{aligned}
$$

That is, using Eqs. (67) and (68),

$$\begin{aligned} A^{-1}(12\bar3\bar4)\frac{\delta M(\bar3\bar4)}{\delta A(34)} &= \beta\left[\frac{\delta M(12)}{\delta g(\bar3)}\right]_q [g(3)\,q(\bar34) + g(4)\,q(\bar33)] \\ &+ \beta\left[\frac{\delta M(12)}{\delta q(\bar3\bar4)}\right]_g [q(\bar33)\,q(\bar44) + q(\bar34)\,q(\bar43)] \\ &+ \beta\left[\frac{\delta M(12)}{\delta g(\bar3)}\right]_q q(\bar35)\,A(56\bar5\bar6)\left[\frac{\delta M(\bar5\bar6)}{\delta g(7)}\right]_q q(74)\,q(63) \end{aligned}$$

and multiplying to the left by A, Eq. (69) follows.

APPENDIX C. DERIVATION OF EQ. (14)

From the definition (72) and (73) of X and P and the expansion for A we have

$$\begin{aligned} P(123) &= A(12\bar1\bar2)\,X(\bar1\bar23) \\ &= X(123) + \Xi(12\bar1\bar2)\,q(\bar15)\,q(\bar26)\{\delta(5-\bar3)\,\delta(6-\bar4) \\ &\quad + \Xi(5678)\,q(7\bar3)\,q(84) + \cdots\}\,X(\bar3\bar43) \\ &= X(123) + \{\Xi(12\bar1\bar2) + \Xi(12\bar5\bar6)\,q(\bar55)\,q(\bar66)\,\Xi(56\bar1\bar2) \\ &\quad + \cdots\}\,q(\bar1\bar3)\,q(\bar2\bar4)\,X(\bar3\bar43) \end{aligned}$$

and observing that the quantity in the brace adds up to Γ, we obtain Eq. (74)

APPENDIX D. LUTTINGER–WARD FREE ENERGY

An arbitrary diagram for Φ contains interaction vertices B, g lines, and q lines. Therefore Φ depends on A only through g and q.

Differentiating Eq. (87) with respect to $A(12)$, we obtain

$$\begin{aligned} \frac{\delta(-\beta W)}{\delta A(12)} &= -\beta\mu(\bar1)\frac{\delta g(\bar1)}{\delta A(12)} - \beta g(1)\,g(2) - 2\beta A(\bar1\bar2)\,g(\bar2)\frac{\delta g(\bar1)}{\delta A(12)} - \beta q(12) \\ &- \beta A(\bar1\bar2)\frac{\delta q(\bar1\bar2)}{\delta A(12)} + \frac{1}{2}q^{-1}(\bar1\bar2)\frac{\delta q(\bar1\bar2)}{\delta A(12)} + \frac{1}{2}\beta\left[\frac{\delta\Phi}{\delta g(\bar1)}\right]_q\frac{\delta g(\bar1)}{\delta A(12)} \\ &+ \left[\frac{\delta\Phi}{\delta q(\bar1\bar2)}\right]_g\frac{\delta q(\bar1\bar2)}{\delta A(12)} \end{aligned}$$

Using Eq. (88), the above expression becomes

$$\begin{aligned} \frac{\delta(-\beta W)}{\delta A(12)} &= \beta[-2A(\bar1\bar2)\,g(\bar2) + \mu(\bar1) + K(\bar1)]\frac{\delta g(\bar1)}{\delta A(12)} \\ &- \frac{1}{2}[2\beta A(\bar1\bar2) - M(\bar1\bar2) - q^{-1}(\bar1\bar2)]\frac{\delta q(\bar1\bar2)}{\delta A(12)} \\ &- \beta[g(1)\,g(2) + q(12)] \end{aligned}$$

Comparing with Eqs. (42) and (52), the quantities in the brackets vanish and we finally have

$$\delta(-\beta W)/\delta A(12) = -\beta[g(1)\,g(2) + q(12)] \tag{D.1}$$

On the other hand, considering the partition function Z given in Eq. (35), we have

$$\delta(\log Z)/\delta A(12) = \langle\delta(-\beta L)/\delta A(12)\rangle = \langle\delta(-\beta G)/\delta A(12)\rangle$$

Using Eqs. (34) and (39), we may compute the above derivative explicitly:

$$\begin{aligned}\delta(\log Z)/\delta A(12) = {}& -\beta[g(1)\,g(2) + q(12)] \\ & -\beta\{2A(\bar{1}\bar{2})\,g(\bar{2}) - \mu(\bar{1}) + 4B(\bar{1}\bar{2}34)[g(\bar{2})\,g(3)\,g(4) \\ & + 3g(\bar{2})\,q(34) + q(\bar{2}34)]\}[\delta g(\bar{1})/\delta A(12)].\end{aligned} \tag{D.2}$$

Comparing with Eqs. (41) and (42), we obtain the same result as in Eq. (D.1):

$$\delta(\log Z)/\delta A(12) = -\beta[g(1)\,g(2) + q(12)]$$

Similarly, differentiating Eq. (87) with respect to B, we obtain

$$\begin{aligned}\frac{\partial(-\beta W)}{\partial B} = {}& \beta\mu(1)\frac{\partial g(1)}{\partial B} - 2\beta A(12)\,g(2)\frac{\partial g(1)}{\partial B} - \beta A(12)\frac{\partial q(12)}{\partial B} \\ & + \frac{1}{2}q^{-1}(12)\frac{\partial q(12)}{\partial B} + \frac{1}{2}\beta\frac{\partial \Phi}{\partial B}\end{aligned} \tag{D.3}$$

In order to compute the derivative of Φ with respect to B, we employ a transformation of the type used by Baym in Ref. 10. A given nth-order diagram for Φ contains n interaction vertices and $2n$ lines, counting two g lines as one. Thus, we may eliminate the explicit B dependence by means of the transformation

$$g \to \bar{g} = B^{1/4}g, \qquad q \to \bar{q} = B^{1/2}q \tag{D.4}$$

Namely, Φ depends on B only through $\bar{g}$ and $\bar{q}$. Varying B, now we shall have

$$\frac{\partial\Phi}{\partial B} = \left[\frac{\delta\Phi}{\delta\bar{g}(1)}\right]_{\bar{q}}\frac{\partial\bar{g}(1)}{\partial B} + \left[\frac{\delta\Phi}{\delta\bar{q}(12)}\right]_{\bar{g}}\frac{\partial\bar{q}(12)}{\partial B} \tag{D.5}$$

Next we note that from Eq. (88) we have

$$\begin{aligned}\left[\frac{\delta\Phi}{\delta\bar{g}(1)}\right]_{\bar{q}} &= B^{-1/4}\left[\frac{\delta\Phi}{\delta g(1)}\right]_{q} = 2B^{-1/4}K(1) \\ \left[\frac{\delta\Phi}{\delta\bar{q}(12)}\right]_{\bar{g}} &= B^{-1/2}\left[\frac{\delta\Phi}{\delta q(12)}\right]_{g} = \beta^{-1}B^{-1/2}M(12)\end{aligned} \tag{D.6}$$

while from Eq. (D.4) it follows that

$$\frac{\partial \bar{g}(1)}{\partial B} = \frac{1}{4} B^{-3/4} g(1) + B^{1/4} \frac{\partial g(1)}{\partial B}$$
$$\frac{\partial \bar{q}(12)}{\partial B} = \frac{1}{2} B^{-1/2} q(12) + B^{1/2} \frac{\partial q(12)}{\partial B} \tag{D.7}$$

Thus, inserting Eqs. (D.6) and (D.7) into Eq. (D.5), we obtain

$$\frac{\partial \Phi}{\partial B} = \frac{1}{2} B^{-1} K(1)\, g(1) + 2K(1) \frac{\partial g(1)}{\partial B} + \frac{1}{2} \beta^{-1} B^{-1} M(12)\, q(12) + \beta^{-1} M(12) \frac{\partial q(12)}{\partial B} \tag{D.8}$$

Inserting, in turn, this result in the r.h.s. of Eq. (D.3) and using again Eqs. (42) and (52), we obtain

$$\frac{\partial(-\beta W)}{\partial B} = \beta[\mu(1) - 2A(12)\, g(2) - K(1)] \frac{\partial g(1)}{\partial B} - \frac{1}{2} [2\beta A(12) - q^{-1}(12) - M(12)] \frac{\partial q(12)}{\partial B} + \tfrac{1}{4}\beta B^{-1} K(1)\, g(1) + \tfrac{1}{4} B^{-1} M(12)\, q(12)$$

i.e.,

$$\partial(-\beta W)/\partial B = \tfrac{1}{4}\beta B^{-1}[K(1)\, g(1) + \beta^{-1} M(12)\, q(12)] \tag{D.9}$$

From Eqs. (41) and (51), for a point interaction, we have

$$K(1)\, g(1) = -4B[g^4(1) + 3g^2(1)\, q(11) + g(1)\, q(111)]$$
$$M(12)\, q(12) = -4\beta B[3g^2(1)\, q(11) + 3q^2(11) + 3g(1)\, q(111) + q(1111)]$$

where the above notation means that all the arguments of the cumulants are taken at the same point and an integration over the volume of the system is understood.

Therefore, Eq. (D.9) can be rewritten as

$$\partial(-\beta W)/\partial B = -\beta[g^4(1) + 6g^2(1)\, q(11) + 3q^2(11) + 4g(1)\, q(111) + q(1111)] \tag{D.10}$$

The corresponding derivative of $\log Z$ is given by

$$\begin{aligned}\frac{\partial(\log Z)}{\partial B} &= \frac{\partial(-\beta L)}{\partial B} + \left\langle \frac{\partial(-\beta G)}{\partial B} \right\rangle \\ &= -\beta\{2A(12)\, g(2) - \mu(1) + 4B[g^3(1) + 3g(1)\, q(11) + q(111)]\} \frac{\partial g(1)}{\partial B} \\ &\quad - \beta[g^4(1) + 6g^2(1)\, q(11) + 3q^2(11) + 4g(1)\, q(111) + q(1111)]\end{aligned}$$

where the last of Eqs. (39) was used.

Comparing with Eqs. (41) and (42), the coefficient of $\partial g(1)/\partial B$ vanishes and we obtain

$$\partial(\log Z)/\partial B = -\beta[g^4(1) + 6g^2(1)\,q(11) + 3q^2(11) + 4g(1)\,q(111) + q(1111)] \tag{D.11}$$

which is the same as Eq. (D.10).

Finally, for the variation of the free energy with respect to β, we make very similar considerations. We note that the quantity $\beta\Phi$ is dimensionless. Thus, the nth-order diagrams for $\beta\Phi$ must contain a factor β^n. In other words, $\beta\Phi$ depends on the temperature explicitly through this factor β^n and implicitly through the β dependence of g and q.

By means of the transformation

$$g \to \bar{g} = \beta^{1/4}g, \qquad q \to \bar{q} = \beta^{1/2}q \tag{D.12}$$

we absorb the explicit temperature dependence into the g and q lines. The effect on $\beta\Phi$ of a variation of β will then be given by

$$\frac{\partial(\beta\Phi)}{\partial\beta} = \left[\frac{\delta(\beta\Phi)}{\delta\bar{g}(1)}\right]_{\bar{q}}\frac{\partial\bar{g}(1)}{\partial\beta} + \left[\frac{\delta(\beta\Phi)}{\delta\bar{q}(12)}\right]_{\bar{g}}\frac{\partial\bar{q}(12)}{\partial\beta} \tag{D.13}$$

On the other hand, from Eq. (D.12) we obtain the set of relations

$$\left[\frac{\delta(\beta\Phi)}{\delta\bar{g}(1)}\right]_{\bar{q}} = \beta^{-1/4}\left[\frac{\delta(\beta\Phi)}{\delta g(1)}\right]_{q} = 2\beta^{3/4}K(1)$$

$$\left[\frac{\delta(\beta\Phi)}{\delta\bar{q}(12)}\right]_{\bar{g}} = \beta^{-1/2}\left[\frac{\delta(\beta\Phi)}{\delta q(12)}\right]_{g} = \beta^{-1/2}M(12)$$

$$\frac{\partial\bar{g}(1)}{\partial\beta} = \frac{1}{4}\beta^{-3/4}g(1) + \beta^{1/4}\frac{\partial g(1)}{\partial\beta}$$

$$\frac{\partial\bar{q}(12)}{\partial\beta} = \frac{1}{2}\beta^{-1/2}q(12) + \beta^{1/2}\frac{\partial q(12)}{\partial\beta}$$

Thus, Eq. (D.13) becomes

$$\frac{\partial(\beta\Phi)}{\partial\beta} = \frac{1}{2}K(1)\,g(1) + \frac{1}{2}\beta^{-1}M(12)\,q(12) + 2\beta K(1)\frac{\partial g(1)}{\partial\beta} + M(12)\frac{\partial q(12)}{\partial\beta}.$$

Taking the derivative with respect to β of Eq. (87), we then obtain

$$\begin{aligned}\frac{\partial(-\beta W)}{\partial\beta} = {} & [\beta\mu(1) - 2\beta A(12)\,g(2) + \beta K(1)]\frac{\partial g(1)}{\partial\beta} \\ & + [\beta A(12) - \tfrac{1}{2}q^{-1}(12) + \tfrac{1}{2}M(12)]\frac{\partial q(12)}{\partial\beta} \\ & + [\mu(1) - A(12)\,g(2) + \tfrac{1}{2}K(1)]\,g(1) \\ & + [\tfrac{1}{2}\beta^{-1}M(12) - A(12)]\,q(12)\end{aligned}$$

i.e., using Eqs. (42) and (52),

$$\partial(-\beta W)/\partial\beta = [\mu(1) - A(12)g(2) + \tfrac{1}{4}K(1)]\,g(1) + [\tfrac{1}{4}\beta^{-1}M(12) - A(12)]\,q(12) \tag{D.14}$$

Differentiating $\log Z$ with respect to β we obtain

$$\begin{aligned}
\frac{\partial(\log Z)}{\partial\beta} &= \frac{\partial(-\beta L)}{\partial\beta} + \left\langle\frac{\partial(-\beta G)}{\partial\beta}\right\rangle \\
&= -\beta\{2A(12)\,g(2) - \mu(1) \\
&\quad + 4B(1234)[g(2)\,g(3)\,g(4) + 3g(2)\,q(34) + q(234)]\}\,\frac{\partial g(1)}{\partial\beta} \\
&\quad - \{A(12)\,g(2) - \mu(1) + \tfrac{1}{4}4B(1234)[g(2)\,g(3)\,g(4) + 3g(2)\,q(34) \\
&\quad + q(234)]\}\,g(1) - \{A(12)\,q(12) + \tfrac{1}{4}4B(1234)[3g(1)\,g(2)\,q(34) \\
&\quad + 3g(1)\,q(234) + q(1234)]\}
\end{aligned}$$

In the above expression the coefficient of $\partial g(1)/\partial\beta$ vanishes as can be seen from Eqs. (41) and (42). The rest of the expression, on comparing it with Eqs. (41) and (51), is seen to reduce to

$$\frac{\partial(\log Z)}{\partial\beta} = [\mu(1) - A(12)\,g(2) + \tfrac{1}{4}K(1)]\,g(1) + [\tfrac{1}{4}\beta^{-1}M(12) - A(12)]\,q(12) \tag{D.15}$$

which is the same as Eq. (D.14).

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