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Statistical mechanics of one-dimensional Ginzburg–Landau fields: Feynman graph evaluation of the screening approximation (n^{-1} expansion)

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Abstract. The free energy per component of an isotropic one-dimensional Ginzburg–Landau field with n components is calculated to order n^{-2} by evaluating the appropriate Feynman graphs. The result agrees with that of Ferrell and Scalapino, obtained by solving the equivalent anharmonic oscillator problem, but the method has greater generality.

1. Introduction

The exact solution of the statistical mechanics of a one-dimensional Ginzburg–Landau (GL) field with n components is well known (Gruenberg and Gunther 1972, Scalapino *et al* 1972). The free energy density is identified with the quantum-mechanical ground state energy of an n-dimensional anharmonic oscillator. Analytic continuation on n may be performed in a straightforward manner (Balian and Toulouse 1974) and a solution obtained for arbitrary n.

In two and three dimensions no such exact solutions exist and one has to fall back on various expansion schemes whereby one expands about an exactly soluble limit in powers of a small parameter which measures the deviation from that limit. One such expansion is the n^{-1} expansion (Abe 1972, 1973a, Ferrell and Scalapino 1972a, b) or 'screening approximation' in which one expands about the Hartree (or 'spherical model') limit $n = \infty$. At the present time the n^{-1} expansion has been carried to second order in three dimensions (Abe 1973b) and to first order in two dimensions (Scalapino *et al* 1973). The *modus operandi* for these expansions is the standard Feynman graph technique by means of which graphs for thermodynamic functions may be conveniently grouped according to their order in $1/n$.

In recent papers, Ferrell and Scalapino (1974a, b, the latter to be referred to as FS) test the $1/n$ expansion by comparing its predictions with the known exact results in one dimension. Working with the equivalent anharmonic oscillator problem they calculate the free energy per component of the order parameter to order n^{-2}, and compare with the exact numerical result for $n = 2$. They find that the first screening approximation (order n^{-1}) provides a marked improvement on the Hartree result with the second screening approximation (order n^{-2}) providing a further modest improvement. In the present paper we recover the FS results by evaluating the appropriate Feynman graphs. Our motivation is the following: for all its elegance the equivalent anharmonic oscillator method is limited strictly to the one-dimensional problem whereas the Feynman graph

technique is valid for arbitrary dimensionality. In particular it should be possible to repeat the present calculation for the interesting two-dimensional case, though the calculation details are admittedly much more involved. We believe, however, that the present paper lays the basis for such a calculation.

2. Hartree and first screening approximations

The statistical mechanics of an isotropic D-dimensional GL field with n components $\Phi_i(x)$ is governed by the following partition function:

$$Z = \int \prod_{i,k} (\mathrm{d}\Phi_i(k)) \exp(-F\{\Phi_i\}) \tag{2.1}$$

where we have introduced the Fourier transformed variables $\Phi_i(k) = \int \mathrm{d}x\, \mathrm{e}^{\mathrm{i}k\cdot x}\Phi_i(x)$ in terms of which the free energy functional F has the canonical form:

$$F\{\Phi_i\} = \tfrac{1}{2}\sum_{i,k}(\tau + k^2)\Phi_i(k)\Phi_i(-k) + \frac{1}{4n}\sum_{\substack{i,j\\k,p,q}} \Phi_i(k)\Phi_i(q-k)\Phi_j(-p)\Phi_j(p-q). \tag{2.2}$$

Here $\tau \propto (T - T_c)/T_c$, where T_c is the mean field transition temperature, and we have set the volume of the system equal to unity. The order parameter correlation function, or propagator, $g(k)$ is given by

$$g(k) = \langle \Phi_j(k)\Phi_j(-k)\rangle \equiv \frac{1}{Z}\int \prod_{i,k} (\mathrm{d}\Phi_i(k))\Phi_j(k)\Phi_j(-k)\exp(-F\{\Phi_i\}). \tag{2.3}$$

We define in the usual way an 'unperturbed' or 'bare' propagator $g_0(k)$ by neglecting the fourth-order term in F whereupon the functional integrations in equations (2.1) and (2.3) factor into products of Gaussian integrals to give

$$g_0(k) = \frac{1}{\kappa_0^2 + k^2}, \qquad \kappa_0^2 = \tau \tag{2.4}$$

Here κ_0^{-1} is the bare correlation length for fluctuations of the order parameter field. It becomes infinite at $\tau = 0$, the mean field transition temperature. The exact or 'dressed' propagator $g(k)$ is given by the standard Feynman graph expansion (Bray 1973) as the sum of all topologically distinct linked graphs with two external lines. The n^{-1} expansion is derived by noting that each interaction vertex has a factor n^{-1} while each closed loop has a factor n arising from a sum over the n components of the order parameter field. Hence graphs can be readily grouped according to their order in n^{-1}. To zeroth order we sum all graphs with equal numbers of interaction vertices and closed loops. The resulting Hartree propagator is given graphically in figure 1 where single and double

Figure 1. Graphical equation for the Hartree propagator $g(k)$. A single full line represents the bare propagator $g_0(k)$.

full lines represent bare and Hartree propagators respectively. The latter satisfies

$$g(k) = g_0(k) - g_0(k)\sum_{k'} g(k')g(k) = \left(\kappa_0^2 + k^2 + \sum_{k'} g(k')\right)^{-1} = (\kappa^2 + k^2)^{-1} \quad (2.5)$$

where

$$\kappa^2 = \kappa_0^2 + \sum_{k'} (\kappa^2 + k'^2)^{-1}. \quad (2.6)$$

In one dimension we can make the replacement

$$\sum_{k'} \to \frac{1}{2\pi}\int_{-\infty}^{\infty} dk'$$

giving

$$\kappa^2 = \kappa_0^2 + \frac{1}{2\kappa}, \quad (2.7)$$

the usual Hartree result. The quantity κ^{-1} is the Hartree correlation length and remains finite for all values of $\kappa_0^2 = \tau$, $-\infty < \tau < \infty$.

We are interested in calculating the free energy $F = -\ln Z$. First we note that the entropy $S = -\partial F/\partial\tau = \partial \ln Z/\partial\tau$ is given very simply by differentiating inside the functional integral equation (2.1):

$$S = -\tfrac{1}{2}\sum_{i,k} \langle \Phi_i(k)\Phi_i(-k)\rangle = -\tfrac{1}{2}n\sum_k g(k).$$

Hence the Hartree free energy per component of the order parameter is

$$f^{(0)} = -\frac{1}{n}\int S\, d\tau = \int \kappa_0\, d\kappa_0 \sum_k g(k) = \int d\kappa \left(\frac{1}{2} + \frac{1}{8\kappa^3}\right) = \tfrac{1}{2}\kappa - \frac{1}{16\kappa^2} \quad (2.8)$$

where equation (2.7) was used to relate κ_0 to κ and the constant of integration was chosen zero to give the correct limit, $f^{(0)} \to \frac{1}{2}\kappa_0 + O(\kappa_0^{-2})$ as $\kappa_0 \to \infty$, which follows from a direct perturbation expansion. Equation (2.8) is identical to equation (3.7) of FS.

The exact free energy per component of the order parameter is given by an expansion of the form

$$f = f^{(0)} + n^{-1}f^{(1)} + n^{-2}f^{(2)} + \ldots.$$

The functions $f^{(1)}, f^{(2)}, \ldots$ may be calculated directly from the graphs for the free energy. These are the usual set of topologically distinct linked graphs with no external lines. As always when evaluating graphs for the free energy, one must divide the contribution of a given graph G by the appropriate symmetry factor, which is usually just the rotational symmetry of the graph.

Since the total free energy is $F = nf = nf^{(0)} + f^{(1)} + n^{-1}f^{(2)} + \ldots$, the graphs for $f^{(1)}$ are those with equal numbers of interaction vertices and closed loops. They are given in figure 2 where single full lines now represent Hartree propagators. The graph

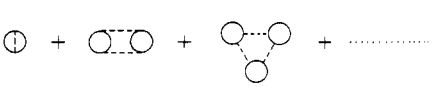

Figure 2. Graphs for $f^{(1)}$, the order n^{-1} contribution to the free energy (per component). A single full line represents the Hartree propagator $g(k)$.

with r loops clearly has rotational symmetry r; also each loop has 'internal' symmetry 2 giving

$$f^{(1)} = \sum_{r=1}^{\infty} \frac{1}{2r} \sum_{q} (-1)^{r+1} \left(\sum_{k} g(k)g(k+q) \right)^{r} = \tfrac{1}{2} \sum_{q} \ln(1+\pi_0(q)) \tag{2.9}$$

where

$$\pi_0(q) = \sum_{k} g(k)g(k+q) = \frac{1}{\kappa} \frac{1}{4\kappa^2+q^2}. \tag{2.10}$$

Substituting into equation (2.9) gives

$$f^{(1)} = \frac{1}{4\pi} \int_{-\infty}^{\infty} \mathrm{d}q \ln\left(1+\frac{1}{\kappa} \frac{1}{4\kappa^2+q^2}\right) = \tfrac{1}{2}(\kappa_2 - 2\kappa) \tag{2.11}$$

where

$$\kappa_2^2 = 4\kappa^2 + \frac{1}{\kappa}. \tag{2.12}$$

Equation (2.11) is identical to equation (5.11) of FS. In two dimensions $f^{(1)}$ has been evaluated by Scalapino *et al* (1973) and in three dimensions, close to the critical point, by Ferrell and Scalapino (1972b).

3. The second screening approximation

We turn now to the calculation of $f^{(2)}$. This consists of graphs with one more interaction vertex than closed loop. Since the insertion of an arbitrary number of polarization loops into a dotted line does not change the order in $1/n$ we are led to introducing a 'screened potential' (Ferrell and Scalapino 1972a, b, Bray and Rickayzen 1972) represented by a wavy line and associated with a factor $-(1/n)\,v(q)$ where

$$v(q) = 1 - \pi_0(q) + \pi_0^2(q) \ldots = (1+\pi_0(q))^{-1}. \tag{3.1}$$

In one dimension equations (2.10) and (2.12) give

$$v(q) = (4\kappa^2+q^2)/(\kappa_2^2+q^2). \tag{3.2}$$

In terms of the screened potential there are four graphs which contribute to $f^{(2)}$. These are given in figure 3. As before a single full line represents the Hartree propagator $g(k) = (\kappa^2+k^2)^{-1}$. Denoting the contributions (apart from sign) of the graphs by $n^{-1}f_{(a)}$, $n^{-1}f_{(b)}$, $n^{-1}f_{(c)}$ and $n^{-1}f_{(d)}$ we have

$$f^{(2)} = -f_{(a)} - \tfrac{1}{2}f_{(b)} + f_{(c)} + \tfrac{2}{3}f_{(d)}. \tag{3.3}$$

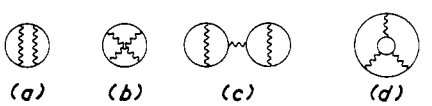

Figure 3. Graphs for $f^{(2)}$, the order n^{-2} contribution to the free energy (per component). A single full line represents the Hartree propagator, a wavy line the screened potential.

The coefficients of the four terms (apart from sign) derive from the reciprocals of the rotational symmetries of the graphs, $\frac{1}{2}, \frac{1}{4}, \frac{1}{2}, \frac{1}{3}$ respectively together with an overall factor 2 coming from a simple counting argument. The quantities $f_{(a)} \ldots f_{(d)}$ are given by

$$f_{(a)} = \sum_{k,p,q} v(p)v(q)g^2(k)g(k+p)g(k+q) \tag{3.4a}$$

$$f_{(b)} = \sum_{k,p,q} v(p)v(q)g(k)g(k+p)g(k+q)g(k+p+q) \tag{3.4b}$$

$$f_{(c)} = v(0)\left(\sum_{kq} v(q)g^2(k)g(k+q)\right)^2 \tag{3.4c}$$

$$f_{(d)} = \sum_{p,q} v(p)v(q)v(p-q)\left(\sum_{k} g(k)g(k+p)g(k+q)\right)^2. \tag{3.4d}$$

The remainder of this section is concerned with the evaluation of these integrals for the one-dimensional case. Since the algebraic details are fairly involved we will just outline the main steps and state the results. Where the phrase 'after simplification' occurs it will usually mean that equation (2.12), relating κ_2 to κ, has been used to obtain the stated result. We consider the graphs in order of complexity, taking the simplest first.

(*i*) *Evaluation of* $f_{(c)}$. We first compute the subsum

$$A(q) = \sum_{k} g^2(k)g(k+q) \tag{3.5}$$

by recognizing that

$$A(q) = -\frac{1}{4\kappa}\frac{\mathrm{d}}{\mathrm{d}\kappa}\pi_0(q) = \frac{12\kappa^2+q^2}{4\kappa^3(4\kappa^2+q^2)^2}.$$

The expression in large parentheses in equation (3.4*c*) is then

$$\sum_{q} v(q)A(q) = \frac{1}{4\kappa^3}\sum_{q}\frac{12\kappa^2+q^2}{(4\kappa^2+q^2)(\kappa_2^2+q^2)} = \frac{1}{2\kappa}+\frac{\kappa_2}{8\kappa^2}-\frac{3}{2\kappa_2}.$$

Using $v(0) = 4\kappa^2/\kappa_2^2$ (equation (3.2)) gives, after simplification

$$f_{(c)} = \frac{1}{16\kappa^4\kappa_2^4}+\frac{1}{2\kappa^2\kappa_2^3}-\frac{4\kappa(\kappa_2-2\kappa)}{\kappa_2^4} \tag{3.6}$$

(*ii*) *Evaluation of* $f_{(a)}$. One may compute the subsum

$$B(k) = \sum_{p} v(p)g(p+k)$$

by noticing that its Fourier transform satisfies $B(x) = v(x)g(x)$ where

$$v(x) = \delta(x)-(1/2\kappa\kappa_2)\exp(-\kappa_2|x|)$$

and $g(x) = (1/2\kappa)\exp(-\kappa|x|)$ are the Fourier transforms of the screened potential and Hartree propagator respectively. This leads to

$$B(k) = \frac{1}{2\kappa}-\frac{1}{2\kappa^2\kappa_2}\frac{\kappa+\kappa_2}{(\kappa+\kappa_2)^2+k^2}$$

Finally $f_{(a)}$ is given by $\Sigma_k\, g^2(k)B^2(k)$ yielding, after simplification,

$$f_{(a)} = \frac{1}{16\kappa^4\kappa_2^4}+\frac{1}{2\kappa^2\kappa_2^3}+\frac{(\kappa_2-2\kappa)^2}{16\kappa^2\kappa_2^4(\kappa+\kappa_2)} \tag{3.7}$$

(*iii*) *Evaluation of* $f_{(d)}$. We compute first the subsum represented by the term in large parentheses (equation 3.4*d*)). Following Abe we call this

$$I(p, q) = \sum_k g(k)g(k+p)g(k+q).$$

This is the point at which difficulties arise in higher dimensionalities, connected with the fact that the summand depends on two angles. This difficulty may be overcome in three dimensions by using the well known Feynman trick (Abe 1973b). In one dimension the sum may be performed by elementary methods to give

$$I(p, q) = \frac{1}{\kappa} \frac{12\kappa^2 + p^2 + q^2 - pq}{(4\kappa^2 + p^2)(4\kappa^2 + q^2)[4\kappa^2 + (p-q)^2]}.$$

Equation (3.4*d*) becomes

$$f_{(d)} = \sum_{p,q} v(p)v(q)v(p-q)I^2(p, q)$$

$$= \frac{1}{\kappa^2} \sum_{p,q} \frac{(12\kappa^2 + p^2 + q^2 - pq)^2}{(\kappa_2^2 + p^2)(\kappa_2^2 + q^2)[\kappa_2^2 + (p-q)^2](4\kappa^2 + p^2)(4\kappa^2 + q^2)[4\kappa^2 + (p-q)^2]}$$

To evaluate this sum we replace $p-q$ by a new variable k, introducing at the same time a Kronecker delta $\delta_{p-q,k}$ and summing over k. Use of the integral representation of the Kronecker delta,

$$\delta_{p-q,k} = \int_{-\infty}^{\infty} \mathrm{d}x \, \mathrm{e}^{\mathrm{i}(p-q-k)x},$$

yields

$$f_{(d)} = \frac{1}{\kappa^2} \int_{-\infty}^{\infty} \mathrm{d}x \sum_{p,q,k} \frac{[12\kappa^2 + \frac{1}{2}(k^2 + p^2 + q^2)]^2 \, \mathrm{e}^{\mathrm{i}(p-q-k)x}}{(\kappa_2^2 + p^2)(\kappa_2^2 + q^2)(\kappa_2^2 + k^2)(4\kappa^2 + p^2)(4\kappa^2 + q^2)(4\kappa^2 + k^2)}$$

where the term in square brackets has been symmetrized with respect to k, p, q by use of the Kronecker delta. This term may be squared out and the sums over k, p, q performed independently by separating the various summands into partial fractions. Finally the integration over x is performed giving, after simplification,

$$f_{(d)} = 3\left(\frac{32\kappa^5(\kappa_2 - 2\kappa) - 4\kappa^2(4\kappa - \kappa_2) + 1}{16\kappa^3\kappa_2^4(\kappa + \kappa_2)}\right) \tag{3.8}$$

(*iv*) *Evaluation of* $f_{(b)}$. We finally consider $f_{(b)}$. This can be written

$$f_{(b)} = \sum_{p,q} v(p)v(q)I_b(p, q)$$

where

$$I_b(p, q) = \sum_k g(k)g(k+p)g(k+q)g(k+p+q).$$

As pointed out by Abe (1973b) we can use the following identity:

$$\kappa^2 + k^2 + \kappa^2 + (k+p+q)^2 - [\kappa^2 + (k+p)^2] - [\kappa^2 + (k+q)^2] = 2pq$$

to express $I_b(p, q)$ in terms of $I(p, q)$ thus:

$$I_b(p, q) = (I(p, q) - I(p, -q)/pq$$
$$= \frac{2}{\kappa} \frac{20\kappa^2 + p^2 + q^2}{(4\kappa^2 + p^2)(4\kappa^2 + q^2)[4\kappa^2 + (p+q)^2][4\kappa^2 + (p-q)^2]}.$$

The sum for $f_{(b)}$ may now be evaluated by a similar technique to that used for $f_{(d)}$: we replace $p+q$ by k, $p-q$ by k', multiply by $\delta_{p+q,k}\delta_{p-q,k'}$ and sum over k and k'. Introduction of the integral representations

$$\delta_{p+q,k} = \int \mathrm{d}x \exp[\mathrm{i}(p+q-k)x],$$

$$\delta_{p-q,k'} = \int \mathrm{d}y \exp[\mathrm{i}(p-q-k')y]$$

is followed by summation over p, q, k and k'. Finally, x and y are integrated over to yield, after simplification,

$$f_{(b)} = \frac{(\kappa_2 - 2\kappa)(\kappa_2 + 10\kappa)}{8\kappa\kappa_2^2(\kappa_2 + \kappa)}. \tag{3.9}$$

Combining equations (3.6)–(3.9) according to equation (3.3) yields the final result

$$f^{(2)} = \frac{12\kappa^2}{\kappa_2^4} - \frac{6}{\kappa_2^3} + \frac{1}{4\kappa\kappa_2^4} \tag{3.10}$$

which is precisely equation (6.33) of FS.

4. Discussion

As noted by FS, inclusion of the second-order screening correction modestly improves the accuracy of the approximation for $n = 2$. (This choice of n corresponds to the superconductor for which the GL theory should provide a good model on account of the long range, $\xi(0)$, of the forces.) For the simpler zero-dimensional case, Bray (1974) has carried the expansion to order n^{-5}. He finds that the accuracy of the approximation improves at first as more terms are included but then ultimately begins to deteriorate. This suggests that the expansion is asymptotic. The number of terms which should be included to give the greatest accuracy then depends on the value of n. Bray finds that including five terms (ie up to n^{-4}) gives the greatest accuracy for $n = 2$, indicating that for $n \geqslant 2$ inclusion of terms at least up to order n^{-3} should be worthwhile in the higher dimensionalities.

Of particular interest is the two-dimensional case for which our knowledge of the phase transition (if indeed one exists in the usual sense) is very limited. For $n \geqslant 2$ general theorems (Mermin and Wagner 1966, Hohenberg 1967) show that there can be no long-range order for any finite temperature, that is $\langle \Phi_i \rangle = 0$ for all finite τ. However, high temperature expansions (Stanley and Kaplan 1966, Stanley 1967, 1968a, b, Moore 1969) indicate a divergence in the susceptibility $\langle \Phi_i(q)\Phi_i(-q)\rangle_{q=0}$ at some non-zero temperature T_c. It has therefore been conjectured (Stanley and Kaplan 1966) that there may be a qualitative change in the range of order at T_c. If this is accompanied by a non-analyticity in the free energy the $1/n$ expansion may give some clue as to its nature.

The order n^{-1} contribution to the free energy has been calculated by Scalapino *et al* (1973) and gives rise to a weak maximum in the specific heat (for all n). It would be of interest to compute the order n^{-2} contribution. We believe that the present paper lays the basis for such a calculation. This is an interesting problem for the future.

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