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Helicity modulus at low temperatures

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Abstract. The helicity modulus (superfluid density) is evaluated for spin systems in the magnon regime and for an interacting Bose fluid in the Bogoliubov approximation. The quantal XY model and the Bose system each yield the same temperature dependence for the helicity modulus; the behaviour is distinct from that of the square of the order parameter.

1. Introduction

In systems with continuous symmetry suitable wall potentials or boundary conditions can induce in the ordered phase a 'twist' in which the order parameter $\Psi(\mathbf{x})$ has a direction which varies in a continuous manner from one end of the system to the other. Such a situation corresponds to a state of superflow in a superfluid or to a Bloch wall in an isotropic magnet. The *helicity modulus* Y(T), as discussed in detail by Fisher *et al* (1973), is a measure of the response of the system to a 'phase twisting' field; in a superfluid the helicity modulus is simply related to the superfluid density according to $\rho_s(T) = (m/\hbar)^2 Y(T)$.

As noted by Fisher *et al* (1973), the helicity modulus can be calculated (at least in principle) within the framework of equilibrium statistical mechanics. One must, however, be prepared to go beyond the bulk properties in the same sense as in a computation of surface properties such as the surface tension. One operational definition of the helicity modulus that has been successfully applied to the Berlin-Kac (1952) spherical model (Barber and Fisher 1973) and to the ideal Bose gas (Barber 1977) involves equilibrium free energy calculations under periodic ($\tau = 0$) and antiperiodic ($\tau = \frac{1}{2}$) boundary conditions:

$$Y(T) = \lim_{L \to \infty} (2L^2/\pi^2) (F^{1/2}(T;L) - F^0(T;L)).$$
(1.1)

Here F^{τ} is the free energy per unit volume of a system infinite in (d-1) dimensions and of length L in the final dimension. (In ordinary space one imagines circular disc geometry with radius $R \to \infty$ before the height L.) The two free energy densities differ by $O(L^{-2})$ when helicity effects are present.

In each of the cases mentioned the helicity modulus can be calculated exactly and one finds for all $T < T_c$

$$Y(T) \propto \begin{cases} M_0(T)^2 & \text{(spherical model)} \\ n_0(T) & \text{(ideal Bose gas)} \end{cases}$$
(1.2)

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(Barber and Fisher 1973, Barber 1977), where $M_0(T)$ is the spontaneous magnetisation and $n_0(T)$ is the condensate density. In each of these cases Y is proportional to $(\Psi_0(T))^2$, the square of the spontaneous order; for the Bose gas one in fact has $\rho_s = mn_0(T)$. This proportionality is special to these related simple models.

An alternative operational definition has been used by Rudnick and Jasnow (1977) to show that the Josephson (1966) relation is exact within the renormalisation group framework. Using a combination of phenomenological and scaling ideas Josephson suggested that as $\Delta T = T - T_c \rightarrow 0 -$, the helicity modulus (superfluid density) behaves as $\Upsilon(T) \sim |\Delta T|^{2\beta - n\nu}$, which is in general distinct from $(\Psi_0(T))^2 \sim |\Delta T|^{2\beta}$. Boundary conditions on the basic variables are difficult to include within usual renormalisation group approaches, so Rudnick and Jasnow imagined that the boundary conditions induce a long-wavelength twist of wavenumber k_0 in the order parameter. The thermodynamic limit is to be taken first, and then the helicity modulus becomes

$$\Upsilon(T) = [\partial^2 F(T; k_0) / \partial k_0^2]_{k_0 = 0}, \qquad (1.3)$$

where $F(T; k_0)$ is the free energy density associated with such an ordered state.

In this paper we apply the general procedure embodied in (1.3) to the XY model in the magnon regime and to the Bogoliubov model for an interacting Bose fluid. One finds for both of these models $Y(T) = A - BT^{d+1} + \dots (d > 2)$, which temperature dependence is in agreement with the phenomenological prediction of Landau (1941, 1947). Such temperature dependence is distinct from that of the order parameter which is well known to behave for these models as $(\Psi_0(T))^2 \sim C - DT^{d-1}$. The results are consistent with the use of the XY model as a lattice model for a Bose fluid (see, e.g., Fisher 1967). Our results for the Bogoliubov model are in agreement with those of Kehr (1967) who uses a formalism specifically designed for a Bose fluid. We include also results for the ideal Bose gas which shows that the definition (1.3) yields precise agreement with the work of Barber (1977) using the alternative and perhaps more fundamental definition (1.1).

The layout is as follows: $\S 2$ deals with the spin systems and $\S 3$ with the boson systems. Several concluding remarks are made in $\S 4$.

2. The XY model

The XY model is defined by the Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} \left[J_{ij} (S_i^x S_j^x + S_i^y S_j^y) + J_{ij}' S_i^z S_j^z \right]$$
(2.1)

where the spins S_i occupy the sites of a (hyper)cubic lattice. We assume that the alignment at low temperatures is ferromagnetic in the xy spin plane; accordingly we take $J_{ij} > |J'_{ij}| \ge 0$. At low temperatures we assume a 'helical' state with a twist is set up so that

$$\langle S_i^x \rangle = M_0 \cos(\mathbf{k}_0 \cdot \mathbf{R}_i), \qquad \langle S_i^y \rangle = M_0 \sin(\mathbf{k}_0 \cdot \mathbf{R}_i), \qquad \langle S_i^z \rangle = 0, \qquad (2.2)$$

where M_0 is the magnitude of the spontaneous order and k_0 is the pitch of the spiral. It is convenient to study the system in a rotating reference frame defined by the

canonical transformation

$$S_i^{z'} = S_i^{z}$$

$$S_i^{e} = -S_i^{x} \sin(\mathbf{k}_0 \cdot \mathbf{R}_i) + S_i^{y} \cos(\mathbf{k}_0 \cdot \mathbf{R}_i)$$

$$S_i^{n} = S_i^{x} \cos(\mathbf{k}_0 \cdot \mathbf{R}_i) + S_i^{y} \sin(\mathbf{k}_0 \cdot \mathbf{R}_i)$$
(2.3)

so that at each site \mathbf{R}_i the magnetisation points in the $\hat{\mathbf{n}}$ -direction. Substitution of the transformed variables into \mathcal{H} yields $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_c$ given by

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} \{ J_{ij} (S_i^n S_j^n + S_i^e S_j^e) \cos [\mathbf{k}_0 \cdot (\mathbf{R}_i - \mathbf{R}_j)] + J'_{ij} S_i^z S_j^z \}$$

$$-\frac{1}{2} \sum_{i,j} J_{ij} \sin [\mathbf{k}_0 \cdot (\mathbf{R}_i - \mathbf{R}_j)] (S_i^n S_j^e - S_i^e S_j^n), \qquad (2.4)$$

which has new features. The first term (\mathcal{H}_0) represents an XY model with an exchange correction, while the second (\mathcal{H}_c) represents a 'current' term (Rudnick and Jasnow 1977). Nonetheless usual spin-wave analysis can be carried out; spin deviations

$$S_{i}^{n} \simeq S - a_{i}^{T} a_{i},$$

$$S_{i}^{+} = S_{i}^{e} + iS_{i}^{z} \simeq (2S)^{1/2} a_{i},$$

$$S_{i}^{-} = S_{i}^{e} - iS_{i}^{z} \simeq (2S)^{1/2} a_{i}^{\dagger},$$
(2.5)

with the *a* and a^{\dagger} boson operators can be introduced, and only quadratic terms are kept in \mathcal{H}_0 . Standard techniques (see, e.g., Kittel 1963, Keffer 1966) can be used to bring it to diagonal form.

The current yields a trilinear term

$$\mathscr{H}_{c} = -i(S/8N)^{1/2} \sum_{k,k'} (\hat{J}_{k+k_{0}} - \hat{J}_{k_{0}-k}) (a_{k}^{\dagger} a_{k'}^{\dagger} a_{k+k'} - a_{k} a_{k'}^{\dagger} a_{k'-k})$$
(2.6)

where, as usual,

$$\hat{J}_{k} = \sum_{i} J_{ij} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_{i}-\boldsymbol{R}_{i})}$$

$$a_{k} = N^{-1/2} \sum_{i} a_{i} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_{i}}$$
(2.7)

and N is the number of spins. In lowest-order spin-wave theory there is a temptation to neglect this term (\mathcal{H}_c) . Indeed a careful analysis indicates that it yields a term $O(T^{2d-1})$ to Y(T) and (for d > 2) is of higher order than the exchange correction noted above. It is the specific nature of the Bogoliubov transformation in the longwavelength limit which makes a potential T^{2d-2} contribution vanish.

The free energy contribution from \mathcal{H}_0 follows from standard techniques; evaluating the helicity modulus according to (1.3) yields a contribution of the form $Y = A - BT^{d+1}$ with A and B positive non-universal constants depending on dimensionality and, for example, on the full Brillouin zone shape. Several additional steps are included in appendix 1. Note in particular that the spontaneous magnetisation has the form

$$N^{-1}\sum_{i} \langle S_{i}^{x} \rangle \equiv m_{0}(T) = m_{0}(0) - m_{1}T^{d-1}, \qquad (2.8)$$

where $0 < m_0(0) \le S$ and $m_1 > 0$ are non-universal constants.

The same sort of analysis can be applied to the Heisenberg model, even though this (n = 3) model is not expected to exhibit a 'twisted' state over a significant time scale. As discussed by Fisher *et al* (1973), it is too easy for an isotropic system with $n \ge 3$ components to untwist, so that a dynamically stable twisted state is not expected. Nonetheless the incremental free energy can be calculated, and one finds for d > 2 as $T \rightarrow 0$,

$$\Upsilon(T) \propto m_0(T) \simeq S - m_1 T^{d/2}.$$
 (2.9)

3. Bose particle systems

We consider first the case of the ideal Bose gas to show that the definition (1.3) yields results in precise agreement with those of Barber (1977) using the (perhaps more fundamental) definition (1.1). The Hamiltonian is written in second quantised form in terms of the Bose field operators $\psi(\mathbf{x})$. A twist is induced by making the transformation $\overline{\psi}(\mathbf{x}) = e^{-ik_0 \cdot \mathbf{x}} \psi(\mathbf{x})$ in complete analogy with (2.3). In terms of the transformed variables the Hamiltonian takes the form ($\hbar = 1$)

$$\mathcal{H} = \frac{1}{2m} \sum_{\boldsymbol{k}} (\boldsymbol{k} + \boldsymbol{k}_0)^2 b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}} - \sum_{\boldsymbol{k}} \bar{\mu} b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}}$$
(3.1)

where the *b* are the usual momentum space operators. The chemical potential $\bar{\mu}$ has to be chosen to preserve particle number, but since the transformation leaves the particle density unchanged we have $\bar{\mu} \rightarrow 0$ characterising the condensed phase.

Note that the equilibrium state would be described by a uniform system of macroscopic occupation of the 'mode' $-\mathbf{k}_0$, in agreement with results in the original frame of reference. However we are interested in the excess free energy due to the imposition of a twisted state. In this language we must consider the effects of the two perturbations,

$$\mathscr{H}' = \sum_{\boldsymbol{k}} (k_0^2/2m) b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}} \quad \text{and} \quad \mathscr{H}'' = \sum_{\boldsymbol{k}} (\boldsymbol{k} \cdot \boldsymbol{k}_0/m) b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}}, \quad (3.2)$$

the second again having the form of a current correction. Perturbation theory is a simple exercise, and one finds

$$\Delta F = k_0^2 n_0(T) / 2m, \tag{3.3}$$

where $n_0(T)$ is the condensate density in the equilibrium system. This leads to the result $\rho_s = (m/\hbar)^2 \Upsilon(T) = mn_0(T)$ in precise agreement with the results of Barber (1977). Using (1.3) in place of (1.1) yields a far simpler calculation, however.

The interest here, however, is to apply the approach to a system of interacting bosons. We can do this within the Bogoliubov approximation (see, e.g., Landau and Lifshitz 1969) for a weakly interacting Bose fluid. The results are expected to be correct asymptotically as $T \rightarrow 0$. In this case we expect, and indeed find, that $\rho_s(T) \neq n_0(T)$.

The Hamiltonian (with $\hbar = 1$) is taken to be of the usual form,

$$\mathscr{H}_{0} = \sum_{k} \frac{k^{2}}{2m} b_{k}^{\dagger} b_{k} + \frac{U_{0}}{2V} \sum_{k_{1}, k_{2}, k_{3}} b_{k_{1}}^{\dagger} b_{k_{2}}^{\dagger} b_{k_{3}} b_{k_{1}+k_{2}-k_{3}}, \qquad (3.4)$$

where V is the volume of the system. Imposition of a twist as above merely replaces

the kinetic energy term by $(\mathbf{k} + \mathbf{k}_0)^2 / 2m$; for convenience we use the same variables, b and b^+ , for the transformed system. One again must evaluate perturbation corrections using (3.2) around the Hamiltonian (3.4). One finds that the excess free energy can be written in the form

$$V \Delta F = \frac{k_0^2}{2m} \sum_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle_0 - \frac{\beta}{2} \sum_{\mathbf{k}, \mathbf{k}'} \frac{(\mathbf{k} \cdot \mathbf{k}_0)(\mathbf{k}' \cdot \mathbf{k}_0)}{m^2} \chi(\mathbf{k}, \mathbf{k}')$$
(3.5)

where $n_k \equiv b_k^{\dagger} b_k$ and

$$\chi(\boldsymbol{k},\boldsymbol{k}') \equiv \beta^{-1} \int_0^\beta \mathrm{d}\lambda \left(\langle n_{\boldsymbol{k}}(\lambda) n_{\boldsymbol{k}'} \rangle_0 - \langle n_{\boldsymbol{k}} \rangle_0 \langle n_{\boldsymbol{k}'} \rangle_0 \right)$$
(3.6)

is the appropriate response function. As usual $X(\lambda)$ denotes the Heisenberg operator, $X(\lambda) = \exp(\lambda \mathcal{H}_0) X \exp(-\lambda \mathcal{H}_0)$, and (3.4) governs the evolution and the averages in (3.6). If one considers only the first term on the right of (3.5) one finds from (1.3) $Y(T) = (\hbar^2/m)n$ where n = N/V is the particle density. This yields a contribution to the superfluid density $\rho_s = (m/\hbar)^2 Y = \rho$, equal to the total mass density. In the twofluid picture the second term on the right of (3.5) corresponds to the normal fluid density.

Of course, we cannot evaluate (3.5) exactly as was possible for the ideal Bose gas. However, for the weakly interacting case at low temperatures, the Bogoliubov approximation can be made. The basic assumption is that at low temperatures the condensate *fraction* is nearly unity; there is some depletion of the ground state, but it is treated as small. Under these circumstances an approximate evaluation of (3.5) can be made. In the Bogoliubov approximation the Hamiltonian \mathcal{H}_0 in (3.4) is replaced by a bilinear operator \mathcal{H}_B . Within this approximation the current type perturbation commutes with \mathcal{H}_B so that much of the complexity of (3.6) is eliminated. The steps are quite familiar so we merely sketch the results.

The Bogoliubov Hamiltonian is

$$\mathscr{H}_{\mathrm{B}} = E_0 + \sum_{k \neq 0} \epsilon(k) C_k^{\dagger} C_k$$
(3.7)

where the C_k are boson operators, E_0 is a constant and

$$\boldsymbol{\epsilon}(\boldsymbol{k}) = [u^2 k^2 + (k^2/2m)^2]^{1/2}, \qquad u^2 = n U_0/m, \qquad (3.8)$$

with *n* the total particle density. At small wavenumbers the excitation spectrum is linear, with slope *u*. To evaluate (3.5) and (3.6) we must re-express the particle opeators $n_k \equiv b_k^{\dagger} b_k$ in terms of the quasi-particle operators C_k and C_k^{\dagger} . This again is straightforward; the operators become λ -independent, and averages with respect to (3.7) decouple in the usual fashion. At low temperatures only the small-*k* part of the spectrum contributes, and one finds for the leading behaviour in d = 3

$$\Delta F = (k_0^2/2m)[n - 2\pi^2/(45\beta^4 u^5 m)]$$
(3.9)

which leads to

$$\rho_{\rm s} = mn - 2\pi^2 (k_{\rm B}T)^4 / 45u^5 \tag{3.10}$$

in agreement with the phenomenological results of Landau (1941, 1947). (Generalisations for d>2 are straightforward; the second term in (3.10) is proportional to T^{d+1} .) Note that the condensate density is given in the Bogoliubov approximation by

$$n_0(T) = n_0(0) - n_1 T^2$$
 in $d = 3$. (3.11)

The results (3.10) and (3.11) have been obtained previously by Kehr (1967, 1969) in a formulation specific to Bose particles and strongly influenced by two-fluid model considerations.

4. Summary and final comments

Fisher et al (1973) suggested a method for calculating the helicity modulus (superfluid density) based entirely on 'beyond the bulk' equilibrium statistical mechanics. To apply the approach one has to evaluate free energy densities in the thermodynamic limit in the presence of specified sort-ranged 'wall potentials'. This seems to us to be the most fundamental definition proposed, but it is extremely difficult to apply it to specific problems. Barber and Fisher (Barber 1977, Barber and Fisher 1973) maintained the spirit of the general definition but calculated the helicity modulus for the ideal Bose gas and spherical models by specifying the boundary conditions on the underlying basic variables: $\psi(x, y, z+L) = \pm \psi(x, y, z)$ for the Bose field operators and $S(\mathbf{R} + L\hat{z}) = S(\mathbf{R})$ for the (lattice) spherical model. Anti-periodic boundary conditions induce a twist in the order parameter which vanishes in the thermodynamic limit.

Even with this simplification (using boundary conditions instead of wall potentials to induce a twist) the approach is difficult to apply to more general interacting systems. It is also difficult to incorporate proper boundary conditions into a conventional renormalisation group approach. Rudnick and Jasnow (1977) showed that by further modifying the definition of the helicity modulus (to (1.3)) a renormalisation group calculation could be carried out. Notice that in (1.3) the thermodynamic limit is taken *first*, then the pitch of the twist is reduced to zero. The difference between the definitions of Y is quite analogous to different definitions of long-range order.

This group of short computations was undertaken with two main objectives. The first was to show that by modifying the definition of the helicity modulus to that given in (1.3), the arsenal of reliable approximate methods could be brought to bear on such calculations. Indeed the form (1.3) is very close to the two-fluid picture. In the second place we demonstrate the generality of the approach and conceptual basis by including the calculation for the XY model at low temperatures. As expected the temperature dependence agrees with that for the Bose particle system. In particular the temperature dependence of the helicity modulus is distinct from that of the square of the order parameter.

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Appendix 1

Substitution of spin deviations (2.7) into (2.4) and retaining only bilinear terms (consistent with usual lowest-order spin-wave analysis) yields

$$\mathcal{H}_{0} \simeq C + \sum_{k} A_{k} a_{k}^{\dagger} a_{k} + \frac{1}{2} \sum_{k} (B_{k} a_{k} a_{-k} + B_{k} a_{k}^{\dagger} a_{-k}^{\dagger}), \qquad (A.1)$$

where

$$C = -\frac{1}{2}NS^{2}\hat{J}_{k_{0}}$$

$$A_{k} = S[\hat{J}_{k_{0}} - \frac{1}{2}J'_{k} - \frac{1}{4}(\hat{J}_{k_{0}+k} + \hat{J}_{k_{0}-k})]$$

$$B_{k} = -\frac{1}{4}S(2J'_{k} - \hat{J}_{k_{0}+k} - \hat{J}_{k_{0}-k}).$$
(A.2)

The Bogoliubov transformation yields quasiparticle energies

$$\epsilon(\mathbf{k}) = S[\hat{J}_{\mathbf{k}_0} - \frac{1}{2}(\hat{J}_{\mathbf{k}_0 + \mathbf{k}} + \hat{J}_{\mathbf{k}_0 - \mathbf{k}})]^{1/2}(\hat{J}_{\mathbf{k}_0} - J'_{\mathbf{k}})^{1/2}$$
(A.3)

in terms of which one has free energy density $F(k_0)$,

$$Va^{-d}F(k_0) = C - \frac{1}{2}\sum_{k} A_k + \frac{1}{2}\sum_{k} (A_k^2 - |B_k|^2)^{1/2} + k_{\rm B}T\sum_{k} \ln[1 - \exp(-\beta\epsilon(k))].$$
(A.4)

As usual sums are restricted to the first Brillouin zone, and $V = Na^d$ with a the lattice spacing. Differentiation with respect to k_0 yields the helicity modulus according to (1.3). The first three terms in (A.4) yield a positive temperature-independent contribution. This is a non-universal value (corresponding to Y(T = 0)) which depends, for example, on the zone shape and the relative strength of \hat{J}'_k . The final term in (A.4) yields (in d = 3) a contribution, $-BT^4$, to the helicity modulus with B positive and non-universal.

From (A.1) and (A.2) with $k_0 = 0$ one evaluates the temperature dependence of the spontaneous order

$$m_0(T) = N^{-1} \sum_i \langle S_i^x \rangle \simeq S - N^{-1} \sum_i \langle a_i^\dagger a_i \rangle$$
(A.5)

for the ordinary XY model. The expectation value in (A.5) is evaluated according to (A.1) with $k_0 = 0$. One finds, as is well known, a depletion from perfect alignment even at T = 0. Such depletion is also non-universal. The leading temperature dependence is universal and one has the leading terms (d = 3),

$$m_0(T) \simeq m_0(0) - m_1 T^2,$$
 (A.6)

where m_1 is also non-universal.

One expects that at low temperatures spin-wave interactions yield a higher-order temperature dependence to Y(T) as well as to the spontaneous magnetisation. Using, for example, the Dyson-Maleev transformation (see, e.g., Silberglitt and Harris 1968) to go beyond linear spin-wave theory indicates that this is indeed the case.

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