



**Übungen zu Zeitabhängige Phänomene
 in der Statistischen Physik
 Sommer Semester 2006**

Übungsblatt 3: Hydrodynamics II and Debye-Waller Factor

Rotors on a lattice II. In the previous problems sheet we considered a simple model for Hydrodynamics consisting of rotors on lattice sites. We considered only the disordered phase but for sufficiently low temperatures the rotors tend to align into an ordered phase reminiscent of the ferromagnetic phase in the Ising model. In addition to the Hydrodynamic modes associated with conserved variables the ordered phase displays an additional slowly varying long wavelength mode. Such additional modes occur quite generally when a continuous symmetry is broken.

In the ordered phase we can consider course graining over a mesoscopic volume to obtain a spacially varying average rotor direction $\mathbf{n}(\mathbf{x}) = [\cos \theta(\mathbf{x}), \sin \theta(\mathbf{x})]$, where $\theta(\mathbf{x})$ is the local average angle. The vector $\mathbf{n}(\mathbf{x})$ is called the director and is zero in the disordered phase. Gradients of $\theta(\mathbf{x})$ give rise to an elastic free energy

$$F_{\text{el}} = \frac{1}{2} \int d\mathbf{x} \rho_s (\nabla \theta(\mathbf{x}))^2,$$

where ρ_s is a stiffness parameter. In order to extend our hydrodynamics to the ordered phase we must include a new thermodynamic variable $\mathbf{v}_\theta(\mathbf{x}) = \nabla \theta(\mathbf{x})$ which has the conjugate variable $\mathbf{h}_\theta(\mathbf{x})$. The appropriate thermodynamic function is

$$W(T, \Omega, [\mathbf{h}_\theta]) = E - \Omega L - TS - \int d\mathbf{x} \mathbf{h}_\theta(\mathbf{x}) \cdot \mathbf{v}_\theta(\mathbf{x}),$$

where $[\cdot]$ indicates a functional dependence. Derive a relation between the intensive quantities $s, \epsilon, l, \mathbf{v}_\theta(\mathbf{x})$. Show that we can expand the Legendre transformed potential $\tilde{W}(T, \Omega, \mathbf{v}_\theta)$ for small \mathbf{v}_θ to obtain

$$\tilde{W}(T, \Omega, \mathbf{v}_\theta) = W(T, \Omega) + F_{\text{el}}(T, \mathbf{v}_\theta).$$

The components of the conjugate field satisfy $h_{\theta i} = -T \left(\frac{\partial s}{\partial v_{\theta i}} \right)_{\epsilon, l} = V^{-1} \left(\frac{\partial \tilde{W}}{\partial v_{\theta i}} \right)_{T, \Omega}$ which give

$h_{\theta i} = \rho_s v_{\theta i}$ to lowest order in \mathbf{v}_θ .

Consider the equation of motion for the angle

$$\frac{d\theta(\mathbf{x})}{dt} + (-\Omega + X') = 0,$$

where we have split the 'current' into two contributions. Why does $X' = 0$ describe the non-dissipative case. We can thus write an equation of motion for \mathbf{v}_θ

$$\frac{\partial \mathbf{v}_\theta}{\partial t} = -\nabla(X' - \Omega).$$

Using this result, the relation between the intensive quantities and the conservation laws for ϵ and l show that the entropy production equation becomes

$$T \left(\frac{\partial s}{\partial t} + \nabla \cdot (\mathbf{Q}/T) \right) = -\mathbf{Q} \cdot (\nabla T/T) - (\mathbf{j}_l + \mathbf{h}_\theta) \cdot \nabla \Omega - X' \nabla \cdot \mathbf{h}_\theta,$$

where the heat/entropy current is given by $\mathbf{Q} = \mathbf{j}_\epsilon - \Omega \mathbf{j}_l - \mathbf{h}_\theta X'$

As was the case in the disordered phase we can postulate constitutive equations for the dissipative parts of the currents

$$\begin{aligned} Q_i &= -\kappa_{ij} \nabla_j T \\ j_{li} &= -h_{\theta i} - \Gamma_{ij} \nabla_j \Omega \\ X' &= -\gamma \nabla \cdot \mathbf{h}_\theta = -\gamma \rho_s \nabla^2 \theta. \end{aligned}$$

In ordered phase the dissipative coefficients become tensors, why? Finally derive the linearized hydrodynamic equations for the ordered phase

$$\begin{aligned} \frac{\partial \epsilon}{\partial t} &= C_l^{-1} \kappa_{ij} \nabla_i \nabla_j \epsilon \\ \frac{\partial \theta}{\partial t} &= \Omega + \gamma \rho_s \nabla^2 \theta = I^{-1} l + \gamma \rho_s \nabla^2 \theta \\ \frac{\partial l}{\partial t} &= \rho_s \nabla \cdot \mathbf{v}_\theta + \Gamma_{ij} \nabla_j \Omega = \rho_s \nabla^2 \theta + I^{-1} \Gamma_{ij} \nabla_i \nabla_j l. \end{aligned}$$

Comment on the coupling between these equations. For the case without dissipation we have that Q_i, j_{li} and X' are all zero. Find the modes of the system in this case.

The Debye-Waller factor. In this problem we will consider scattering of waves from a crystal structure and the effect of motion in the crystal lattice on the intensity of the Bragg peaks. In the early days of x-ray scattering it was not clear whether Bragg peaks would be destroyed or simply reduced by thermal motion, an issue which is closely connected to the presence of long range order in a solid. The Debye-Waller factor describes the effects of temperature on the Bragg peaks and thus is a useful measure of crystalline order.

The scattering cross section of a material (ordered or disordered) is proportional to the correlator of density fluctuations in Fourier space $\langle n(\mathbf{q})n(-\mathbf{q}) \rangle$, where $n(\mathbf{x}) = \sum_i \delta(\mathbf{x} - \mathbf{x}_i)$. By Considering the Ursell function

$$S_{nn}(\mathbf{x}_1, \mathbf{x}_2) = \langle n(\mathbf{x}_1)n(\mathbf{x}_2) \rangle - \langle n(\mathbf{x}_1) \rangle \langle n(\mathbf{x}_2) \rangle$$

show that the scattering cross section is proportional to

$$NS_{nn}(\mathbf{q}) + |\langle n(\mathbf{q}) \rangle|^2.$$

Show also that for a liquid the second term gives a contribution $N^2 \delta_{\mathbf{q},0}$. What is the meaning of this result?

When the sample is crystalline we can imagine the atoms to be located at the sites of a periodic lattice. Show that for a crystal at zero temperature $n(\mathbf{q}) = N \delta_{\mathbf{q},\mathbf{G}}$, where \mathbf{G} is a reciprocal lattice vector. The cross section thus receives a contribution $\sim N^2$ due to constructive interference whenever the probe wavevector $\mathbf{q} = \mathbf{G}$. These are the Bragg peaks. Now consider a finite temperature for which the atoms are slightly displaced from their perfect lattice sites, $\mathbf{r}_i = \mathbf{R}_i + \mathbf{u}_i$, where the lattice sites are at \mathbf{R}_i and small displacements are \mathbf{u}_i . We can express the small displacements as a Fourier sum $\mathbf{u}_i = \sum_{\mathbf{q}} \mathbf{U}_{\mathbf{q}} \exp(-i\mathbf{q} \cdot \mathbf{R}_i)$, where $\mathbf{U}_{\mathbf{q}}$ is the vector amplitude of the mode with wavevector \mathbf{q} . Make a series expansion of $n_{\mathbf{q}}$ in powers of $\mathbf{U}_{\mathbf{q}}$ and look at the behaviour as $\mathbf{q} \rightarrow \infty$ where $\exp(-i\mathbf{q} \cdot \mathbf{R}_i) = 1$. Focus on the dominant contribution to the series $-\frac{1}{2}|\mathbf{k} \cdot \mathbf{U}_{\mathbf{q}}|^2$ to show that in this Gaussian approximation

$$n(\mathbf{k}) = \sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} \exp\left(-\sum_{\mathbf{q}} \frac{k^2}{6} \langle U_{\mathbf{q}} U_{-\mathbf{q}} \rangle\right) = \sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} e^{-W}.$$

W is the Debye-Waller factor. Using elasticity theory it can be shown that the correlation function $\langle U_{\mathbf{q}} U_{-\mathbf{q}} \rangle \sim \frac{1}{q^2}$. What does this suggest about long range order in a two dimensional crystal?