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8.334 Statistical Mechanics II: Statistical Physics of Fields
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II.D Scattering and Fluctuations

In addition to bulk thermodynamic experiments, scattering measurements can be used to probe microscopic fluctuations at length scales of the order of the probe wavelength λ . In a typical set up, a beam of wavevector \mathbf{k}_i is incident upon the sample and the scattered intensity is measured at wavevector $\mathbf{k}_s = \mathbf{k}_i + \mathbf{q}$. For *elastic* scattering, $|\mathbf{k}_i| = |\mathbf{k}_s| \equiv k$, and $q \equiv |\mathbf{q}| = 2k \sin \theta$, where θ is the angle between incident and scattered beams. Standard treatments of scattering start with the Fermi Golden Rule, and usually lead to a scattering amplitude of the form

$$A(\mathbf{q}) \propto \langle \mathbf{k}_s \otimes f | \mathcal{U} | \mathbf{k}_i \otimes i \rangle \propto \sigma(\mathbf{q}) \int d^d \mathbf{x} e^{i\mathbf{q} \cdot \mathbf{x}} \rho(\mathbf{x}). \quad (\text{II.31})$$

In the above expression, $|i\rangle$ and $|f\rangle$ refer to the initial and final states of the microscopic scattering element (the atom or ion), \mathcal{U} is the scattering potential that can be decomposed as a sum due to the various scattering elements in the sample. The amplitude has a *local* form factor $\sigma(\mathbf{q})$ describing the scattering from an individual element. For our purposes, the more interesting *global* information is contained in $\rho(\mathbf{q})$, the Fourier transform of the global density of scatterers $\rho(\mathbf{x})$. The appropriate scattering density depends on the nature of the probe. Light scattering senses the actual atomic density, electron scattering measures the charge density, while neutron scattering is usually used to probe the magnetization density. Most such probes actually do not look at a snapshot of the system, but look at time averaged configurations. Thus the observed scattering intensity is

$$S(\mathbf{q}) \propto \langle |A(\mathbf{q})|^2 \rangle \propto \langle |\rho(\mathbf{q})|^2 \rangle. \quad (\text{II.32})$$

Here $\langle \bullet \rangle$ indicates the thermal average of \bullet , which can be used in place of the time average in most cases due to ergodicity.

Eq.(II.32) indicates that a uniform density only leads to forward scattering ($\mathbf{q} = \mathbf{0}$), while the long-wavelength fluctuations can be studied by working at small angles or with small k . If scattering is caused by the magnetization density, we can use the Landau–Ginzburg Hamiltonian to compute its intensity. The probability of a particular configuration is given by

$$\mathcal{P}[\vec{m}(\mathbf{x})] \propto \exp \left\{ - \int d^d \mathbf{x} \left[\frac{K}{2} (\nabla m)^2 + \frac{t}{2} m^2 + u m^4 \right] \right\}. \quad (\text{II.33})$$

As discussed earlier, the most probable configuration is *uniform*, with $\vec{m}(\mathbf{x}) = \bar{m}\hat{e}_1$, where \hat{e}_1 is a unit vector (\bar{m} is zero for $t > 0$, and equal to $\sqrt{-t/4u}$ for $t < 0$). We can examine small fluctuations around such a configuration by setting

$$\vec{m}(\mathbf{x}) = [\bar{m} + \phi_\ell(\mathbf{x})]\hat{e}_1 + \sum_{\alpha=2}^n \phi_{t,\alpha}(\mathbf{x})\hat{e}_\alpha, \quad (\text{II.34})$$

where ϕ_ℓ and ϕ_t refer to *longitudinal* and *transverse* fluctuations respectively. The latter can take place along any of the $n-1$ directions perpendicular to the average magnetization.

After the substitution of eq.(II.34), the terms appearing in the Landau–Ginzburg Hamiltonian can be expanded to second order as

$$\begin{aligned} (\nabla m)^2 &= (\nabla \phi_\ell)^2 + (\nabla \phi_t)^2, \\ m^2 &= \bar{m}^2 + 2\bar{m}\phi_\ell + \phi_\ell^2 + \phi_t^2, \\ m^4 &= \bar{m}^4 + 4\bar{m}^3\phi_\ell + 6\bar{m}^2\phi_\ell^2 + 2\bar{m}^2\phi_t^2 + \mathcal{O}(\phi_\ell^3, \phi_t^3), \end{aligned}$$

resulting in a quadratic energy cost

$$\begin{aligned} \beta\mathcal{H} \equiv -\ln \mathcal{P} = & V \left(\frac{t}{2}\bar{m}^2 + u\bar{m}^4 \right) + \int d^d\mathbf{x} \left[\frac{K}{2}(\nabla \phi_\ell)^2 + \frac{t + 12u\bar{m}^2}{2}\phi_\ell^2 \right] \\ & + \int d^d\mathbf{x} \left[\frac{K}{2}(\nabla \phi_t)^2 + \frac{t + 4u\bar{m}^2}{2}\phi_t^2 \right] + \mathcal{O}(\phi_\ell^3, \phi_t^3). \end{aligned} \quad (\text{II.35})$$

For uniform distortions, the longitudinal and transverse *restoring potentials* have “spring constants” given by,

$$\frac{K}{\xi_\ell^2} \equiv t + 12u\bar{m}^2 = \left. \frac{\partial^2 \Psi(m)}{\partial \phi_\ell^2} \right|_{\bar{m}} = \begin{cases} t & \text{for } t > 0 \\ -2t & \text{for } t < 0 \end{cases}, \quad (\text{II.36})$$

and

$$\frac{K}{\xi_t^2} \equiv t + 4u\bar{m}^2 = \left. \frac{\partial^2 \Psi(m)}{\partial \phi_t^2} \right|_{\bar{m}} = \begin{cases} t & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases}. \quad (\text{II.37})$$

(The physical significance of the length scales ξ_ℓ and ξ_t will soon become apparent.) Note that there is no distinction between longitudinal and transverse components for the paramagnet ($t > 0$). For the ordered magnet in $t < 0$, there is no restoring force for the transverse fluctuations which correspond to the Goldstone modes discussed in the previous section.

Following the change of variables to the Fourier modes, $\phi(\mathbf{x}) = \sum_{\mathbf{q}} \phi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}/\sqrt{V}$, the probability of a particular fluctuation configuration is given by

$$\mathcal{P} [\{\phi_{\ell,\mathbf{q}}; \phi_{t,\mathbf{q}}\}] \propto \prod_{\mathbf{q}} \exp \left\{ -\frac{K}{2}(q^2 + \xi_\ell^{-2})|\phi_{\ell,\mathbf{q}}|^2 \right\} \cdot \exp \left\{ -\frac{K}{2}(q^2 + \xi_t^{-2})|\phi_{t,\mathbf{q}}|^2 \right\}. \quad (\text{II.38})$$

Clearly each mode behaves as a Gaussian random variable of zero mean, and the two point correlation functions are

$$\langle \phi_{\alpha, \mathbf{q}} \phi_{\beta, \mathbf{q}'} \rangle = \frac{\delta_{\alpha, \beta} \delta_{\mathbf{q}, -\mathbf{q}'}}{K(q^2 + \xi_{\alpha}^{-2})}, \quad (\text{II.39})$$

where the indices refer the longitudinal, or any of the transverse components. By using a spin polarized source of neutrons, the relative orientations can be adjusted to probe either the longitudinal or the transverse correlations. The *Lorentzian form*, $S(\mathbf{q}) \propto 1/(q^2 + \xi^{-2})$, usually provides an excellent fit to scattering line shapes away from the critical point. Eq.(II.39) indicates that in the ordered phase, longitudinal scattering still gives a Lorentzian form (on top of a delta-function at $\mathbf{q} = \mathbf{0}$ due to the spontaneous magnetization), while transverse scattering always grows as $1/q^2$. The same power law decay is also predicted to hold at the critical point, $t = 0$. Actual experimental fits yield a power law of the form

$$S(\mathbf{q}, T = T_c) \propto \frac{1}{q^{2-\eta}}, \quad (\text{II.40})$$

with a small positive value of η .

II.E Correlation Functions and Susceptibilities

We can also examine the extent of fluctuations in real space. The averages $\langle \phi_{\alpha}(\mathbf{x}) \rangle = \langle m_{\alpha}(\mathbf{x}) - \bar{m}_{\alpha} \rangle$, are clearly zero, and the *connected correlation function* is

$$\begin{aligned} G_{\alpha, \beta}^c(\mathbf{x}, \mathbf{x}') &\equiv \langle (m_{\alpha}(\mathbf{x}) - \bar{m}_{\alpha})(m_{\beta}(\mathbf{x}') - \bar{m}_{\beta}) \rangle \\ &= \langle \phi_{\alpha}(\mathbf{x}) \phi_{\beta}(\mathbf{x}') \rangle = \frac{1}{V} \sum_{\mathbf{q}, \mathbf{q}'} e^{i\mathbf{q} \cdot \mathbf{x} + i\mathbf{q}' \cdot \mathbf{x}'} \langle \phi_{\alpha, \mathbf{q}} \phi_{\beta, \mathbf{q}'} \rangle. \end{aligned} \quad (\text{II.41})$$

Using eq.(II.39), we obtain

$$G_{\alpha, \beta}^c(\mathbf{x}, \mathbf{x}') = \frac{\delta_{\alpha, \beta}}{V} \sum_{\mathbf{q}} \frac{e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}')}}{K(q^2 + \xi_{\alpha}^{-2})} \equiv -\frac{\delta_{\alpha, \beta}}{K} I_d(\mathbf{x} - \mathbf{x}', \xi_{\alpha}), \quad (\text{II.42})$$

where in the continuum limit,

$$I_d(\mathbf{x}, \xi) = - \int \frac{d^d \mathbf{q}}{(2\pi)^d} \frac{e^{i\mathbf{q} \cdot \mathbf{x}}}{q^2 + \xi^{-2}}. \quad (\text{II.43})$$

Alternatively, I_d is the solution to the following differential equation

$$\nabla^2 I_d(x) = \int \frac{d^d \mathbf{q}}{(2\pi)^d} \frac{q^2 e^{i\mathbf{q} \cdot \mathbf{x}}}{q^2 + \xi^{-2}} = \int \frac{d^d \mathbf{q}}{(2\pi)^d} \left[1 - \frac{\xi^{-2}}{q^2 + \xi^{-2}} \right] e^{i\mathbf{q} \cdot \mathbf{x}} = \delta^d(\mathbf{x}) + \frac{I_d(\mathbf{x})}{\xi^2}. \quad (\text{II.44})$$

The solution is spherically symmetric, satisfying

$$\frac{d^2 I_d}{dx^2} + \frac{d-1}{x} \frac{dI_d}{dx} = \frac{I_d}{\xi^2} + \delta^d(\mathbf{x}). \quad (\text{II.45})$$

We can try out a solution that decays exponentially at large distances as

$$I_d(x) \propto \frac{\exp(-x/\xi)}{x^p}. \quad (\text{II.46})$$

(We have anticipated the presence of a subleading power law.) The derivatives of I_d are given by

$$\begin{aligned} \frac{dI_d}{dx} &= -\left(\frac{p}{x} + \frac{1}{\xi}\right) I_d, \\ \frac{d^2 I_d}{dx^2} &= \left(\frac{p(p+1)}{x^2} + \frac{2p}{x\xi} + \frac{1}{\xi^2}\right) I_d. \end{aligned} \quad (\text{II.47})$$

For $x \neq 0$, the requirement that eq.(II.46) satisfies eq.(II.45) gives

$$\frac{p(p+1)}{x^2} + \frac{2p}{x\xi} + \frac{1}{\xi^2} - \frac{p(d-1)}{x^2} - \frac{(d-1)}{x\xi} = \frac{1}{\xi^2}. \quad (\text{II.48})$$

The choice of ξ as the decay length ensures that the constant terms in the above equation cancel. The exponent p is determined by requiring the next largest terms to cancel. For $x \ll \xi$, the $1/x^2$ terms are the next most important; we must set $p(p+1) = p(d-1)$, and $p = d-2$. This is the familiar exponent for Coulomb interactions, and indeed at this length scale the correlations don't feel the presence of ξ , and decay as

$$I_d(x) \simeq C_d(x) = \frac{x^{2-d}}{(2-d)S_d} \quad (x \ll \xi). \quad (\text{II.49})$$

(Note that a constant term can always be added to the solution to satisfy the limits appropriate to the correlation function under study.) At large distances $x \gg \xi$, the $1/(x\xi)$ term dominates eq.(II.48), and its vanishing implies $p = (d-1)/2$. Matching to eq.(II.49) at $x \approx \xi$ yields

$$I_d(x) \simeq \frac{\xi^{(3-d)/2}}{(2-d)S_d x^{(d-1)/2}} \exp(-x/\xi) \quad (x \gg \xi). \quad (\text{II.50})$$

The length scale ξ is known as the *correlation length*. From eq.(II.42), we observe that transverse and longitudinal correlations behave differently. Close to the critical point, the longitudinal correlation length (eq.(II.36)) behaves as

$$\xi_\ell = \begin{cases} t^{-1/2}/\sqrt{K} & \text{for } t > 0 \\ (-2t)^{-1/2}/\sqrt{K} & \text{for } t < 0 \end{cases}. \quad (\text{II.51})$$

The singularities can be described by $\xi_{\pm} \simeq \xi_0 B_{\pm} |t|^{-\nu_{\pm}}$, where $\nu_{\pm} = 1/2$ and $B_+/B_- = \sqrt{2}$ are universal, while $\xi_0 \propto 1/\sqrt{K}$ is not. The transverse correlation length (eq.(II.37)) equals ξ_{ℓ} for $t > 0$, and is infinite for all $t < 0$.

Eq.(II.49) implies that right at T_c , correlations decay as $1/x^{d-2}$. Actually, the decay exponent is usually indicated by $1/x^{d-2+\eta}$, where η is the same exponent introduced in eq.(II.40). Integrating the connected correlation functions results in bulk susceptibilities. For example, the divergence of the longitudinal susceptibility is also obtained from,

$$\chi_{\ell} \propto \int d^d \mathbf{x} G_{\ell}^c(\mathbf{x}) \propto \int_0^{\xi_{\ell}} \frac{d^d x}{x^{d-2}} \propto \xi_{\ell}^2 \simeq A_{\pm} t^{-1}. \quad (\text{II.52})$$

The universal exponents and amplitude ratios are again recovered from the above equation. For $T < T_c$, there is no upper cut-off length for transverse correlations, and the divergence of the transverse susceptibility can be related to the system size L , as

$$\chi_t \propto \int d^d \mathbf{x} G_t^c(\mathbf{x}) \propto \int_0^L \frac{d^d x}{x^{d-2}} \propto L^2. \quad (\text{II.53})$$

II.F Comparison to Experiments

The true test of the validity of the approach outlined in previous sections is in its comparison with experiments. A table of exponents, and the appropriate experimental materials is provided below.

Transition Type	Material	α	β	γ	ν
Ferromagnets ($n = 3$)	Fe, Ni	-0.1	0.4	1.3	
Superfluid ($n = 2$)	He ⁴	0	0.3	1.3	0.7
Liquid-Gas ($n = 1$)	CO ₂ , Xe	0.1	0.3	1.2	0.7
Ferroelectrics and Superconductors	TGS	0	1/2	1	1/2
Mean-field theory		0	1/2	1	1/2

The exponents are actually known to much better accuracy than indicated in the table. The final row (mean-field theory) refers to the results obtained from the saddle point approximation. They agree only with the experiments on ferroelectric and superconducting materials. The disagreement between the exponents for different values of n suggests that the mean-field results are too universal, and leave out some essential dependence on n (and d). How do we account for these discrepancies? The starting point of the Landau-Ginzburg Hamiltonian is sufficiently general to be trustworthy. The difficulty is in the saddle point method used in the evaluation of its partition function, as will become apparent in the following sections.