8.B. Static Correlation Functions & Response Functions

Read §8.A of Reichl's text.

8.B.1. General Relations

Consider a system of N particles in a container of volume V at fixed temperature T. The i^{th} particle is characterized by its momentum operator $\hat{\boldsymbol{p}}_i$, position operator $\hat{\boldsymbol{q}}_i$ and spin $\hat{\mathbf{s}}_i$, which gives rise to a magnetic moment $\boldsymbol{\mu} = \mu\, \hat{\mathbf{s}}_i$. The magnetization density operator at position $\boldsymbol{r}$ is defined as

$$\hat{\boldsymbol{m}}(\boldsymbol{r}) = \mu \sum_{i=1}^{N} \hat{\mathbf{s}}_i\, \delta(\hat{\boldsymbol{q}}_i - \boldsymbol{r}) \tag{8.1}$$

The total magnetization operator is

$$\hat{\boldsymbol{M}} = \int_V d\,\boldsymbol{r}\, \hat{\boldsymbol{m}}(\boldsymbol{r}) \;= \mu \sum_{i=1}^{N} \hat{\mathbf{s}}_i \tag{8.2}$$

In a magnetic field of induction $\boldsymbol{B}(\boldsymbol{r})$, the Hamiltonian of the system is

$$\hat{H} = \hat{H}_0 - \int_V d\,\boldsymbol{r}\, \hat{\boldsymbol{m}}(\boldsymbol{r}) \cdot \boldsymbol{B}(\boldsymbol{r}) \tag{8.3}$$

where

$$\hat{H}_0 = \sum_{i=1}^{N} \frac{\hat{\boldsymbol{p}}_i^2}{2\,m} + \sum_{i>j} V(\hat{\boldsymbol{q}}_i, \hat{\boldsymbol{q}}_j, \boldsymbol{s}_i, \boldsymbol{s}_j) \tag{8.4}$$

is the unperturbed Hamiltonian.

From now on, we shall assume $\boldsymbol{B}$ is a constant so that (8.3) becomes

$$\hat{H} = \hat{H}_0 - \hat{\boldsymbol{M}} \cdot \boldsymbol{B} \tag{8.4a}$$

The average magnetization is given by

$$\langle \boldsymbol{M} \rangle_{\boldsymbol{B}} = \frac{\mathrm{Tr}\left(e^{-\beta \hat{H}}\, \hat{\boldsymbol{M}} \right)}{\mathrm{Tr}\left(e^{-\beta \hat{H}} \right)} \tag{8.5}$$

Note: The purpose of using the caret ^ is to remind us that quantum operators may not commute. For the average of a single operator $\hat{X}$, the result is just a function and there is no issue of commutativity. Therefore, we shall denote it as $\langle X \rangle$. On the other hand, the average of two operators $\hat{X}$ & $\hat{Y}$ will be denoted as $\left\langle \hat{X}\, \hat{Y} \right\rangle$ since, in general, $\hat{X}\,\hat{Y} \neq \hat{Y}\,\hat{X}$.

Let

$$\hat{\boldsymbol{M}} = \left\{ \hat{M}_\alpha,\;\; \alpha = x, y, z \right\}$$

then (8.4a) gives

$$\frac{\partial\, \hat{H}}{\partial\, B_\alpha} = -\hat{M}_\alpha \tag{8.5a}$$

The static magnetic susceptibility tensor is defined as

$$\chi_{\alpha\,\alpha'} = \left(\frac{\partial\, \langle M_\alpha \rangle_{\boldsymbol{B}}}{\partial\, B_{\alpha'}} \right)_{T,\, N,\, \boldsymbol{B}=0}$$

$$= \left(\frac{\partial}{\partial B_{\alpha'}} \frac{\mathrm{Tr}\left(e^{-\beta \hat{H}} \hat{M}_\alpha \right)}{\mathrm{Tr}\left(e^{-\beta \hat{H}} \right)} \right)_{\boldsymbol{B}=0}$$

$$= \left(\frac{\mathrm{Tr}\left[e^{-\beta \hat{H}} \left(-\beta \frac{\partial \hat{H}}{\partial B_{\alpha'}} \right) \hat{M}_\alpha \right]}{\mathrm{Tr}\left(e^{-\beta \hat{H}} \right)} - \frac{\mathrm{Tr}\left(e^{-\beta \hat{H}} \hat{M}_\alpha \right) \mathrm{Tr}\left[e^{-\beta \hat{H}} \left(-\beta \frac{\partial \hat{H}}{\partial B_{\alpha'}} \right) \right]}{\left[\mathrm{Tr}\left(e^{-\beta \hat{H}} \right) \right]^2} \right)_{\boldsymbol{B}=0}$$

$$= \beta \left(\frac{\mathrm{Tr}\left(e^{-\beta \hat{H}} \hat{M}_{\alpha'} \hat{M}_\alpha \right)}{\mathrm{Tr}\left(e^{-\beta \hat{H}} \right)} - \frac{\mathrm{Tr}\left(e^{-\beta \hat{H}} \hat{M}_\alpha \right) \mathrm{Tr}\left(e^{-\beta \hat{H}} \hat{M}_{\alpha'} \right)}{\mathrm{Tr}\left(e^{-\beta \hat{H}} \right)^2} \right)_{\boldsymbol{B}=0}$$

$$= \beta \left(\left\langle \hat{M}_{\alpha'} \hat{M}_\alpha \right\rangle_0 - \langle M_\alpha \rangle_0 \langle M_{\alpha'} \rangle_0 \right)$$

$$= \beta \left(\left\langle \hat{M}_\alpha \hat{M}_{\alpha'} \right\rangle_0 - \langle M_\alpha \rangle_0 \langle M_{\alpha'} \rangle_0 \right) \qquad [\, \hat{M}_{\alpha'} \hat{M}_\alpha = \hat{M}_\alpha \hat{M}_{\alpha'} \,]$$

$$= \beta \left\langle \left(\hat{M}_\alpha - \langle M_\alpha \rangle_0 \right) \left(\hat{M}_{\alpha'} - \langle M_{\alpha'} \rangle_0 \right) \right\rangle_0 \qquad (8.6)$$

$$= \beta \left\langle \delta \hat{M}_\alpha \, \delta \hat{M}_{\alpha'} \right\rangle_0$$

$$= \chi_{\alpha' \alpha}$$

where

$$\delta \hat{\boldsymbol{M}} = \hat{\boldsymbol{M}} - \langle \boldsymbol{M} \rangle_0 \qquad \delta \hat{M}_\alpha = \hat{M}_\alpha - \langle M_\alpha \rangle_0 \qquad (8.6a)$$

Note: According to (8.5) "^" is omitted inside $\langle\ \rangle$.

Similarly, we set

$$\delta \hat{\boldsymbol{m}}(\boldsymbol{r}) = \hat{\boldsymbol{m}}(\boldsymbol{r}) - \langle \boldsymbol{m}(\boldsymbol{r}) \rangle_0 \qquad \delta \hat{m}_\alpha(\boldsymbol{r}) = \hat{m}_\alpha(\boldsymbol{r}) - \langle m_\alpha(\boldsymbol{r}) \rangle_0$$

to write (8.6) as

$$\chi_{\alpha \alpha'} = \beta \int_V d\boldsymbol{r} \int_V d\boldsymbol{r}' \langle \delta m_\alpha(\boldsymbol{r}) \, \delta m_{\alpha'}(\boldsymbol{r}') \rangle_0$$

$$= \beta \int_V d\boldsymbol{r} \int_V d\boldsymbol{r}' \, C_{\alpha \alpha'}(\boldsymbol{r}, \boldsymbol{r}') \qquad (8.7)$$

where

$$C_{\alpha \alpha'}(\boldsymbol{r}, \boldsymbol{r}') = \left\langle \delta \hat{m}_\alpha(\boldsymbol{r}) \, \delta \hat{m}_{\alpha'}(\boldsymbol{r}') \right\rangle_0 \qquad (8.8)$$

is the spatial correlation function between the magnetization density fluctuations at points r and r'.

For $V \to \infty$, boundary effects can be neglected so that

$$C_{\alpha \alpha'}(\boldsymbol{r}, \boldsymbol{r}') = C_{\alpha \alpha'}(\boldsymbol{r} - \boldsymbol{r}')$$

$$= \left\langle \delta \hat{m}_\alpha(\boldsymbol{r} - \boldsymbol{r}') \, \delta \hat{m}_{\alpha'}(\boldsymbol{0}) \right\rangle_0$$

Setting $\boldsymbol{\rho} = \boldsymbol{r} - \boldsymbol{r}'$ gives

$$C_{\alpha \alpha'}(\boldsymbol{r}, \boldsymbol{r}') = C_{\alpha \alpha'}(\boldsymbol{\rho}) = \left\langle \delta \hat{m}_\alpha(\boldsymbol{\rho}) \, \delta \hat{m}_{\alpha'}(\boldsymbol{0}) \right\rangle_0 \qquad (8.9)$$

and (8.7) becomes

$$\chi_{\alpha \alpha'} = \beta V \int_V d\boldsymbol{\rho} \int_V d\boldsymbol{R} \, C_{\alpha \alpha'}(\boldsymbol{\rho}) \qquad [\, \boldsymbol{R} = \frac{1}{2}(\boldsymbol{r} + \boldsymbol{r}') \,]$$

$$= \beta V \int_V d\boldsymbol{\rho} \; C_{\alpha \alpha'}(\boldsymbol{\rho}) \qquad (8.10)$$

The static structure factor is defined as the Fourier transform of the static correlation function

$$G_{\alpha \alpha'}(\boldsymbol{k}) \equiv \int_V d\boldsymbol{\rho} \, e^{-i \boldsymbol{k} \cdot \boldsymbol{\rho}} \, C_{\alpha \alpha'}(\boldsymbol{\rho}) \qquad (8.11)$$

$$= \frac{1}{V}\int_V d\boldsymbol{\rho}\int_V d\boldsymbol{R}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{\rho}}\, C_{\alpha\alpha'}(\boldsymbol{\rho})$$
$$= \frac{1}{V}\int_V d\boldsymbol{r}\int_V d\boldsymbol{r}'\, e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\langle\, \delta\hat{m}_\alpha(\boldsymbol{r})\,\delta\hat{m}_{\alpha'}(\boldsymbol{r}')\,\rangle_0$$
$$= \frac{1}{V}\langle\, \delta\hat{m}_\alpha(\boldsymbol{k})\,\delta\hat{m}_{\alpha'}(-\boldsymbol{k})\,\rangle_0 \qquad (8.12)$$

where, like (8.11),

$$\delta\hat{m}_\alpha(\boldsymbol{k}) = \int_V d\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\,\delta\hat{m}_\alpha(\boldsymbol{r})$$
$$\rightarrow \qquad \delta\hat{m}_\alpha(\boldsymbol{r}) = \frac{1}{V}\sum_k e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\,\delta\hat{m}_\alpha(\boldsymbol{k}) \qquad (8.13)$$
$$= \int \frac{dk}{(2\pi)^3}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\,\delta\hat{m}_\alpha(\boldsymbol{k}) \qquad [\, V\to\infty\,]$$

Caution: Reichl used $e^{-i\boldsymbol{k}\cdot\boldsymbol{\rho}}$ in (8.11). This difference is a matter of taste and has no physical significance since only functions of $\boldsymbol{r}$ are measurable physical quantities. Thus, $f(\boldsymbol{r})$ must be real but $f(\boldsymbol{k})$ can be complex.

Comparing (8.10) with (8.11), we see that

$$\chi_{\alpha\alpha'} = \beta V G_{\alpha\alpha'}(\boldsymbol{0}) \qquad (8.14)$$

This means the static linear response $\chi_{\alpha\alpha'}$ involves only the infinite wavelength component of the equilibrium fluctuation correlation $C_{\alpha\alpha'}(\boldsymbol{\rho})$.

8.B.2. Application to the Ising Lattice

In the Ising model, the Hamiltonian (8.3) is approximated by [see §7.F]

$$H = \sum_{\langle i,j\rangle} \epsilon_{ij}\, s_i\, s_j - \mu B \sum_i s_i \qquad (8.15a)$$

where $\sum_{\langle i,j\rangle}$ indicates sum over all nearest neighbor pairs. ϵ_{ij} is the magnetic interaction energy between the z-components, s_i and s_j, of the spins at sites i and j, respectively.

Consider a 3-D Ising lattice with volume V, number of sites N, and temperature $T > T_C$ so that $\langle \boldsymbol{M}\rangle = 0$.

We now break the lattice into blocks of volume Δ. Each block thus contains $n = \frac{\Delta}{V} N$ sites (spins). Let the z-component of magnetization in the l^{th} block be m_l. Since

$$m_l = \mu \sum_{j=1}^{n} s_j \qquad s_j = \pm 1 \qquad (8.15b)$$

we have,

$$m_l = -n\mu,\ -(n-1)\mu,\ \ldots,\ (n-1)\mu,\ n\mu \qquad (8.15c)$$

(8.15a) then becomes

$$H = \sum_{\langle l,k\rangle} \tilde{\epsilon}_{lk}\, m_l\, m_\kappa - \mu B \sum_l m_l$$

where $\tilde{\epsilon}_{lk}$ is the effective interaction energy between blocks l and κ.

The partition function of the system is

$$Z(T, B) = \sum_{\{m_l\}} e^{-\beta H} \tag{8.15}$$

where the sum is over all configurations of m_l.

A magnetic system can also be studied In the Ginzburg-Landau mean field theory discussed in §3.G. To begin, we must generalize (3.78) to describe an inhomogeneous system. This is achieved by replacing the homogeneous order parameter η with $\delta m(\boldsymbol{r})$. Assuming an applied field along the z-axis with magnitude B, we write the free energy as

$$\phi(T, B) = \phi(T) - \int_V d\boldsymbol{r}\, \delta m(\boldsymbol{r})\, B$$

$$\phi(T) = a(T) + \frac{1}{2} C_1(T) \int_V d\boldsymbol{r} \left[\delta m(\boldsymbol{r}) \right]^2 \tag{8.16}$$

$$+ \frac{1}{2} C_2(T) \int_V d\boldsymbol{r} \left[\nabla\, \delta m(\boldsymbol{r}) \cdot \nabla\, \delta m(\boldsymbol{r}) \right] + O[\delta m]^4$$

where $a(T)$ is the nonmagnetic free energy. The gradient term is an attempt to describe the spin-spin interaction. However, explicit linkage to the Ising model is difficult to derive. The factors $\frac{1}{2}$ are included to conform with Reichl's results.

The partition function of the system is the path integral

$$Z(T, B) = \int \mathcal{D}\, \delta m(\boldsymbol{r})\, e^{-\beta\, \phi(T,B)} \tag{8.16a}$$

which includes integrations over all values of $\delta m(\boldsymbol{r})$ at every position $\boldsymbol{r}$.

Now,

$$\int_V d\boldsymbol{r} \left[\delta m(\boldsymbol{r}) \right]^2 = \int_V d\boldsymbol{r}\, \frac{1}{V^2} \sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{r}}\, \delta m(\boldsymbol{k})\ \delta m(\boldsymbol{k}')$$

$$= \frac{1}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} \delta_{\boldsymbol{k},-\boldsymbol{k}'}\, \delta m(\boldsymbol{k})\ \delta m(\boldsymbol{k}')$$

$$= \frac{1}{V} \sum_{\boldsymbol{k}} \delta m(\boldsymbol{k})\ \delta m(-\boldsymbol{k}) \tag{8.17}$$

$$\int_V d\boldsymbol{r} \left[\nabla \delta m(\boldsymbol{r}) \right]^2 = \int_V d\boldsymbol{r}\, \frac{1}{V^2} \sum_{\boldsymbol{k},\boldsymbol{k}'} (-\boldsymbol{k}\cdot\boldsymbol{k}')\, e^{i(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{r}}\, \delta m(\boldsymbol{k})\ \delta m(\boldsymbol{k}')$$

$$= \frac{1}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} (-\boldsymbol{k}\cdot\boldsymbol{k}')\, \delta_{\boldsymbol{k},-\boldsymbol{k}'}\, \delta m(\boldsymbol{k})\ \delta m(\boldsymbol{k}')$$

$$= \frac{1}{V} \sum_{\boldsymbol{k}} \boldsymbol{k}^2\, \delta m(\boldsymbol{k})\ \delta m(-\boldsymbol{k}) \tag{8.18}$$

(8.16) thus becomes

$$\phi(T) = a(T) + \frac{1}{2V} \sum_{\boldsymbol{k}} \left(C_1 + \boldsymbol{k}^2 C_2 \right) \delta m(\boldsymbol{k})\ \delta m(-\boldsymbol{k}) + O[\delta m]^4 \tag{8.19}$$

The probability of a fluctuation $\delta m(\boldsymbol{k})$ to occur is therefore [see (7.46)]

$$P[\delta m(\boldsymbol{k})] = C \exp\left\{ -\beta \left[\frac{1}{2V} \left(C_1 + \boldsymbol{k}^2 C_2 \right) \delta m(\boldsymbol{k})\ \delta m(-\boldsymbol{k}) \right] \right\} \tag{8.20a}$$

where C is a normalization constant given by

$$\int d[\delta m(\boldsymbol{k})]\ P[\delta m(\boldsymbol{k})] = 1$$

Note that

$$\int d[\delta m(\boldsymbol{k})] = 2\pi \int_0^\infty d\ \left|\delta m(\boldsymbol{k})\right| \qquad (8.20b)$$

Since $\delta m(\boldsymbol{r})$ is real, (8.13) gives

$$\delta m(\boldsymbol{r}) = \frac{1}{V}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\,\delta m^*(\boldsymbol{k})$$

$$= \frac{1}{V}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\,\delta m^*(-\boldsymbol{k})$$

$$\rightarrow \qquad \delta m^*(-\boldsymbol{k}) = \delta m(\boldsymbol{k})$$

$$\delta m^*(\boldsymbol{k}) = \delta m(-\boldsymbol{k})$$

(8.20a) can therefore be written as

$$P[\delta m(\boldsymbol{k})] = C\exp\left\{-\beta\left[\frac{1}{2V}\left(C_1 + \boldsymbol{k}^2 C_2\right)\left|\delta m(\boldsymbol{k})\right|^2\right]\right\} \qquad (8.20)$$

(8.12) then becomes

$$G(\boldsymbol{k}) = \frac{1}{V}\langle\delta m(\boldsymbol{k})\,\delta m(-\boldsymbol{k})\rangle$$

$$= \frac{1}{V}\int_0^\infty d\ \left|\delta m(\boldsymbol{k})\right|\ P[\delta m(\boldsymbol{k})]\left|\delta m(\boldsymbol{k})\right|^2$$

$$= \frac{1}{\beta\left(C_1 + \boldsymbol{k}^2 C_2\right)} \qquad (8.21)$$

where we have used

$$\frac{\int_0^\infty x^2 e^{-a x^2}\,dx}{\int_0^\infty e^{-a x^2}\,dx} = \frac{1}{2a}$$

(8.14) thus becomes

$$\chi = \frac{V}{C_1} \qquad (8.22)$$

Near a phase transition,

$$\chi \propto \frac{1}{T - T_C}$$

so that

$$C_1 \propto T - T_C$$

The Fourier inverse of (8.11) gives

$$C(\boldsymbol{\rho}) = \frac{1}{V}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{\rho}}\,G(\boldsymbol{k})$$

$$\approx \int \frac{d\boldsymbol{k}}{(2\pi)^3}\,e^{i\boldsymbol{k}\cdot\boldsymbol{\rho}}\,G(\boldsymbol{k})$$

$$
\begin{aligned}
&= \int \frac{d\boldsymbol{k}}{(2\pi)^3} e^{i\boldsymbol{k}\cdot\boldsymbol{\rho}} \frac{1}{\beta\left(C_1 + \boldsymbol{k}^2 C_2\right)} \\
&= \frac{1}{(2\pi)^2} \int_{-1}^{1} d\cos\theta \int_0^\infty dk\, k^2\, e^{ik\rho\cos\theta} \frac{1}{\beta\left(C_1 + k^2 C_2\right)} \\
&= \frac{1}{(2\pi)^2 \beta i \rho} \int_0^\infty dk\, k \frac{e^{ik\rho} - e^{-ik\rho}}{C_1 + k^2 C_2} \\
&= \frac{1}{2\pi^2 \beta \rho} \int_0^\infty dk \frac{k \sin k\rho}{C_1 + k^2 C_2} \\
&= \frac{1}{4\pi\beta\rho C_2} e^{-\rho\sqrt{C_1/C_2}} \qquad (8.23)
\end{aligned}
$$

Mathematica command to get (8.23):

In[1]:= `Assuming[ρ > 0, ∫_0^∞ (k Sin[k ρ])/(c1 + k^2 c2) ⅆk]`

Out[1]= `ConditionalExpression[` $\frac{e^{-\frac{\sqrt{c1}\,\rho}{\sqrt{c2}}}\pi}{2\,c2}$, `Re[` $\frac{\sqrt{c1}}{\sqrt{c2}}$ `] > 0]`

From (8.23), we get the correlation length

$$\xi = \sqrt{\frac{C_2}{C_1}}$$

Since $C_1 \propto T - T_C$ near the critical point,

$$\xi \propto (T - T_C)^{-1/2} \to \infty \qquad \text{as} \qquad T \to T_C$$

which mean that, at the critical point, correlations between fluctuations extends throughout the entire system.