

☞ See W. D. McComb, “**renormalization method, A GUIDE FOR BEGINNERS**”, (Oxford, 2004).

7.4 Linear response theory (Page 160)

This is a method for working out the response function (e.g. the magnetic susceptibility) of a system in thermal equilibrium. It relies on a clever mathematical trick but also has an underlying physical interpretation. For once we shall begin with the mathematical idea and come back to the physics later. In statistical mechanics, we saw that we can work out the mean value of the energy, for instance, $\langle E \rangle$, either directly from the usual expectation value (as in eqn

$$U = \langle E \rangle = \sum_r p_r E_r = \frac{1}{Z} \sum_r E_r e^{-\beta E_r}, \quad Z = \sum_i e^{-\beta E_r}$$

or indirectly by differentiating the partition function with respect to the temperature T , as in eqn

$$U = \frac{1}{Z} \sum_r E_r e^{-\beta E_r} = -\frac{1}{Z} \left(\frac{\partial Z}{\partial \beta} \right)_{\{V\}} = - \left(\frac{\partial (\log Z)}{\partial \beta} \right)_{\{V\}}.$$

In fact, this idea is available as a general technique for any variable X (say) and the general algorithm may be stated as follows:

- Add a fictitious term $-X Y$ to the energy (or Hamiltonian) of the system.
- Work out the partition function Z as a function of Y .
- Differentiate $\ln Z$ with respect to Y and then put $Y = 0$.

That is,

$$\frac{1}{\beta} \left. \frac{\partial \ln Z}{\partial Y} \right|_{Y=0} = \frac{1}{\beta Z} \left. \frac{\partial}{\partial Y} \sum_i e^{-\beta(E_r - X_i Y)} \right|_{Y=0} = \frac{1}{Z} \sum_i X_i e^{-\beta(E_r - X_i Y)} = \langle X \rangle \quad (7.42)$$

So the two methods are equivalent. If we use

$$-\frac{1}{\beta} \ln Z = F$$

from eqn ($Z = e^{-\beta F}$), then the mean value of the variable X follows at once as:

$$\langle X \rangle = - \left. \frac{\partial F}{\partial Y} \right|_{Y=0} \quad (7.43)$$

Then, differentiating again with respect to Y gives the fluctuations in X :

$$\langle X^2 \rangle - \langle X \rangle^2 = \frac{1}{\beta} \left. \frac{\partial \langle X \rangle}{\partial Y} \right|_{Y=0} = \frac{\chi}{\beta} \quad (7.44)$$

where χ is the generalized susceptibility. This is known as the linear response equation.

What is the physical interpretation? Answer: If we apply a field (external) in order to generate the new term in the Hamiltonian, then this applied field breaks the symmetry of the system. In this way, the response of the system to a symmetry-breaking perturbation is revealed.

7.4.1 Example: spins on a lattice

As a specific example, we shall again consider the Ising microscopic model of a ferromagnet, which consists of a lattice of N spins, with a spin vector S_i at each lattice site i . Note that:

$$H = -\varepsilon \sum_{i=1}^{N-1} S_i S_{i+1} \quad \varepsilon > 0, \quad Z_N = \sum_{\{S_i = \pm 1\}} e^{K \sum_{i=1}^{N-1} S_i S_{i+1}}, \quad K = \beta \varepsilon$$

7.4.1.1 *The mean magnetization.* We begin with the mean magnetization, which we

denote by

$$M = \langle S \rangle$$

where

$$S = \sum_{i=1}^N S_i \equiv \text{total spin.}$$

In line with the procedure of the previous section, we add a term

$$\Delta H = \left(-\frac{1}{\beta} \right) JS$$

to the Hamiltonian or energy. (Actually $J = \beta B$, where B is the magnetic field). Then

$$M = \left. \frac{\partial \ln \mathcal{Z}}{\partial J} \right|_{J=0}. \quad (7.45)$$

7.4.1.2 *Correlation functions.* Allow J (or B) to be different at each lattice site: add the term

$$\Delta H' = - \sum_i \frac{J_i S_i}{\beta},$$

to the Hamiltonian. Hence we may obtain the mean and correlations as follows:

$$\langle S_i \rangle = \frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial J_i}, \quad (7.46)$$

$$\langle S_i S_j \rangle = \frac{1}{\mathcal{Z}} \frac{\partial^2 \mathcal{Z}}{\partial J_i \partial J_j}, \quad (7.47)$$

$$\langle S_i S_j S_k \rangle = \frac{1}{\mathcal{Z}} \frac{\partial^3 \mathcal{Z}}{\partial J_i \partial J_j \partial J_k}, \quad (7.48)$$

where $\langle S_i S_j \dots \rangle$ are the *correlations*.

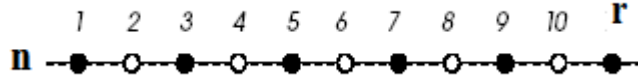
7.4.1.3 *Connected correlations.* We can also treat connected correlations, which (as defined by eqn (7.9)) involve fluctuations about the mean value, in this way and these are generated by differentiating $\ln \mathcal{Z}$, thus:

$$G_c(i, j) = \frac{\partial^2 \ln \mathcal{Z}}{\partial J_i \partial J_j} \quad (7.49)$$

The above is the *pair correlation*: a generalization to the n -point connected correlation is possible:

$$G_c(i_1, \dots, i_N) = \frac{\partial}{\partial J_{i_1}}, \dots, \frac{\partial}{\partial J_{i_N}} \ln \mathcal{Z} \equiv \langle S_{i_1} \dots S_{i_N} \rangle_c. \quad (7.50)$$

Simple calculation: calculate $\langle S_n S_{n+r} \rangle$. Note that $Z_N \approx 2^N \{ \cosh(K) \}^{N-1} = 2^N \prod_{i=1}^{N-1} \cosh(K_i)$



Define

$$G_n(r) = \langle S_n S_{n+r} \rangle$$

where r is the distance between sites, measured in units of lattice constant a . Using:

$$H = -\sum_{i=1}^{N-1} J_i S_i S_{i+1} \quad J > 0, \quad Z_N = \sum_{\{S\}} e^{\sum_{i=1}^{N-1} K_i S_i S_{i+1}}, \quad K_i = \beta J_i$$

$$G_n(r) = \langle S_n S_{n+r} \rangle = \frac{1}{Z_N} \sum_{\{S\}} S_n S_{n+r} e^{\sum_{i=1}^{N-1} K_i S_i S_{i+1}} = \frac{1}{Z_N} \sum_{\{S\}} S_n S_{n+r} e^{K_1 S_1 S_2 + \dots + K_n S_n S_{n+1} + \dots}$$

Re-write

$$Z_N G_n(r) = \frac{1}{Z_N} \sum_{\{S\}} S_n S_{n+r} e^{K_1 S_1 S_2 + \dots + K_n S_n S_{n+1} + \dots}$$

Consider nearest neighbor case: $r=1$

$$Z_N G_n(1) = \sum_{\{S\}} S_n S_{n+1} e^{K_1 S_1 S_2 + \dots + K_n S_n S_{n+1} + \dots} = \frac{\partial}{\partial K_n} \sum_{\{S\}} e^{K_1 S_1 S_2 + \dots + K_n S_n S_{n+1} + \dots} = \frac{\partial}{\partial K_n} Z_N$$

and inductively,

$$Z_N G_n(r) = \frac{\partial}{\partial K_n} \frac{\partial}{\partial K_{n+1}} \dots \frac{\partial}{\partial K_{n+r-1}} Z_N$$

Hence:

$$2^N \prod_{i=1}^{N-1} \cosh(K_i) G_n(1) = 2^N \prod_{i=1}^{N-2} \cosh(K_i) \sinh(K_n)$$

$$\Rightarrow \prod_{i=1}^{N-2} \cosh(K_i) \cosh(K_n) G_n(1) = \prod_{i=1}^{N-2} \cosh(K_i) \sinh(K_n)$$

Therefore

$$G_n(1) = \tanh(K_n), \quad \Rightarrow \quad G_n(r) = \prod_{i=1}^r \tanh(K_{n+i-1})$$

Uniform interaction gives $G_n(r) = \tanh^r(K)$

Consider limit $r \rightarrow \infty$. $T > 0$, $\tanh K < 1$ and $G_n \rightarrow 0$ as $r \rightarrow \infty$. Hence for $T = 0$, $K \rightarrow \infty$ and $G_n \rightarrow 1$.

$$\left. \begin{aligned} \langle S_i S_j \rangle &= \frac{1}{Z} (\cosh K)^{N-1} 2^N (\tanh K)^{|i-j|} = (\tanh K)^{|i-j|}, \\ \langle S_i S_j \rangle &= e^{-|i-j| |\ln \tanh K|} = e^{-|i-j| |\ln \tanh(J/kT)|}. \end{aligned} \right\}$$

Note that: More frequently we will use the relation: $X^A = e^{A \ln X}$