

## Lecture 4

In lecture 3 we defined spin-spin correlation function:

$$G_{ij} = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$$

and demonstrated that it can be evaluated as:

$$G_{ij} = -T \left. \frac{\partial^2 F}{\partial B_i \partial B_j} \right|_{B=0}$$

where the free energy is evaluated for the following Hamiltonian:

$$H = -\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j - \sum_i B_i \sigma_i$$

Now let's consider functional integral representation of the Ising model and calculate  $G_{ij}$  from there.

$$Z = \int D\varphi e^{-S[\varphi]}$$

$$S[\varphi] = \frac{1}{2T} \sum_{ij} \varphi_i J_{ij}^{-1} \varphi_j - \sum_i \ln \left[ 2 \cosh \left( \frac{\varphi_i + B_i}{T} \right) \right]$$

$$G_{ij} = -T \left. \frac{\partial^2 F}{\partial B_i \partial B_j} \right|_{B=0} =$$

$$= T^2 \frac{1}{Z} \left. \frac{\partial^2 Z}{\partial B_i \partial B_j} \right|_{B=0} = T^2 \frac{1}{Z^2} \left. \frac{\partial Z}{\partial B_i} \right|_{B=0} \left. \frac{\partial Z}{\partial B_j} \right|_{B=0}$$

Change variables in the functional integral:

$$\varphi_i \rightarrow \varphi_i - \beta_i$$

Then we obtain:

$$S[\varphi] = \frac{1}{2T} \sum_j (\varphi_i - \beta_i) J_{ij}^{-1} (\varphi_j - \beta_j) - \sum_i \ln [2 \cosh \left( \frac{\varphi_i}{T} \right)]$$

Then we have:

$$\frac{\partial Z}{\partial \beta_i} \Big|_{B=0} = \int D\varphi \left( \frac{1}{T} \sum_j J_{ij}^{-1} \varphi_j \right) e^{-S[\varphi]}$$

Change variables again:

$$m_i = \sum_j J_{ij}^{-1} \varphi_j$$

The physical meaning of variable  $m_i$ , as we will see in a second, is fluctuating magnetization at site  $i$ .

$$S[m] = \frac{1}{2T} \sum_j m_i J_{ij} m_j - \sum_i \ln [2 \cosh \left( \frac{\sum_j J_{ij} m_j}{T} \right)]$$

$$\frac{1}{Z} \left. \frac{\partial Z}{\partial B_i} \right|_{B=0} = \frac{1}{Z} \int Dm \frac{m_i}{T} e^{-S[m]} = \\ = \frac{1}{T} \langle m_i \rangle$$

On the other hand  $\left. \frac{1}{Z} \frac{\partial Z}{\partial B_i} \right|_{B=0} = \langle \sigma_i \rangle$

Thus  $\langle \sigma_i \rangle = \langle m_i \rangle$

Analogously :

$$\frac{1}{Z} \left. \frac{\partial^2 Z}{\partial B_i \partial B_j} \right|_{B=0} = \frac{1}{T^2} \langle m_i m_j \rangle$$

Thus :

$$G_{ij} = \langle m_i m_j \rangle - \langle m_i \rangle \langle m_j \rangle$$

Thus there is a direct correspondence between correlation functions of spins and of the real order-parameter variables in the functional integral representation.

Let us now calculate  $G_{ij}$  in the mean-field approximation.

$$Z = e^{-S[m]}$$

4

$m$  minutes  $S$ .

$$F = -T \ln Z = T S[m] =$$

$$= \frac{1}{2} \sum_j m_j Y_{ij} w_j - T \sum_i \ln \left[ 2 \cosh \left( \frac{\sum_j Y_{ij} w_j + B_i}{T} \right) \right]$$

$$m_i = -\frac{\partial F}{\partial B_i} = T \frac{\partial}{\partial B_i} \ln Z = T \frac{1}{Z} \frac{\partial Z}{\partial B_i}$$

$$m_i = -\frac{\partial F}{\partial B_i} = \tanh \left( \frac{\sum_j Y_{ij} w_j + B_i}{T} \right)$$

$$g_{ij} = -T \frac{\partial^2 F}{\partial B_i \partial B_j} \Big|_{B=0} = T \frac{\partial m_i}{\partial B_j} \Big|_{B=0} = \\ = T \frac{\partial}{\partial B_j} \tanh \left( \frac{\sum_e Y_{ie} m_e + B_i}{T} \right) =$$

$$= \left[ \delta_{ij} + \sum_e Y_{ie} \frac{\partial m_e}{\partial B_j} \Big|_{B=0} \right] \left[ 1 - \tanh^2 \left( \frac{\sum_e Y_{ie} m_e}{T} \right) \right]$$

$$= \left[ \delta_{ij} + \frac{1}{T} \sum_e Y_{ie} g_{ej} \right] \left[ 1 - m^2 \right]$$

~~are concerned in their behavior as  $m$  approaches zero. In fact, they are small compared to 1.~~

Calculate  $g_{ij}$  above  $T_c \Rightarrow m=0$ .

Then we obtain the following equation for  $g_{ij}$ :

$$\sum_k \left[ \delta_{ik} - \frac{1}{L} \delta_{ik} \right] g_{kj} = \delta_{ij}$$

Solve by Fourier transform.

Introduce lattice Fourier transforms:

$$f_i = \frac{1}{N} \sum_k g_{kj} e^{i k \cdot \vec{r}_i}$$

Assume periodic boundary conditions:

$$g(\vec{r}_i) \equiv f_i = g(\vec{r}_i + L \vec{\alpha})$$

where  $L$  is the linear size of the system and

~~the basis vectors~~  $\vec{\alpha}$  are the ~~unit~~ unit vectors along the basis directions of the lattice.

$$\text{This means that } e^{i k \cdot \vec{r}_i} = e^{i k \cdot (\vec{r}_i + L \vec{\alpha})}$$

$$\vec{k} \cdot \vec{\alpha} = k_\alpha = \frac{2\pi n_\alpha}{L}, \text{ where } n_\alpha \text{ is any integer.}$$

$$\vec{r}_i = \sum_{\vec{\alpha}} M_i \alpha \vec{\alpha}, \text{ where } \alpha \text{ is the lattice constant and } M_i \text{ are integers.}$$

This means that  $k_\alpha$  can be restricted to the first BZ:

$$-\frac{\pi}{a} \leq k_x < \frac{\pi}{a}.$$

This is because the shift  $k_x \rightarrow k_x + \frac{2\pi n}{a}$  doesn't change  $\vec{k} \cdot \vec{r}_i$ .

Similarly we can define Fourier transforms of the correlation function  $G_{ij}$  and of the interaction  $J_{ij}$ :

$$G_{ij} = \frac{1}{N} \sum_{\vec{q}} G(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

$$J_{ij} = \frac{1}{N} \sum_{\vec{q}} J(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

Here we explicitly use translational invariance: both  $G_{ij}$  and  $J_{ij}$  only depend on  $\vec{r}_i - \vec{r}_j$ .

Substitute this into the equation for  $G_{ij}$ :

$$G_{ij} - \frac{1}{T} \sum_{\vec{e}} J_{ie} G_{ej} = \delta_{ij}$$

$$\frac{1}{N} \sum_{\vec{q}} G(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} -$$

$$- \frac{1}{T} \sum_{\vec{e}} \frac{1}{N^2} \sum_{\vec{q}_1, \vec{q}_2} J(\vec{q}_1) e^{i\vec{q}_1 \cdot (\vec{r}_i - \vec{r}_e)} G(\vec{q}_2) e^{i\vec{q}_2 \cdot (\vec{r}_e - \vec{r}_j)} =$$

$$= \frac{1}{N} \sum_{\vec{q}} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

Here we've used  $\delta_{ij} = \frac{1}{N} \sum_{\vec{q}} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$

$$\frac{1}{N} \sum_{\vec{q}} e^{-i(\vec{q} \perp \vec{q}^u) \cdot \vec{r}_e} = \delta_{\vec{q}_1, \vec{q}^u}$$

Then we obtain:

$$\begin{aligned} & \frac{1}{N} \sum_{\vec{q}} G(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} - \\ & - \frac{1}{T} \frac{1}{N} \sum_{\vec{q}} \gamma(\vec{q}) G(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} = \\ & = \frac{1}{N} \sum_{\vec{q}} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \end{aligned}$$

Thus we obtain:

$$G(\vec{q}) \left[ 1 - \frac{1}{T} \gamma(\vec{q}) \right] = 1$$

$$G(\vec{q}) = \frac{1}{1 - \frac{1}{T} \gamma(\vec{q})}$$

Calculate  $\mathcal{I}(\vec{q})$ .

$$\mathcal{I}(\vec{q}) = \frac{1}{N} \sum_{ij} J_{ij} e^{-i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

We are interested in the behavior of  ~~$J_{ij}$~~   ~~$J_{ij}$~~  at long distances.

long distances means  ~~$|r_i - r_j| \gg R$~~ , where  $R$  is the effective range of the interaction  $J_{ij}$ .

Typically  $R \sim a$ .

long distances mean small momenta:  $qR \ll 1$ .

Let's calculate  $\mathcal{I}(\vec{q})$  at such small momenta.

In this case we can expand the exponential in the expression for  $\mathcal{I}(\vec{q})$  in Taylor series:

$$\mathcal{I}(\vec{q}) \approx \frac{1}{N} \sum_{ij} J_{ij} \left\{ 1 - i\vec{q} \cdot (\vec{r}_i - \vec{r}_j) - \right. \\ \left. - \frac{1}{2} [i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)]^2 + \dots \right\}$$

clearly, the second term vanishes if  $J_{ij} = J_{ji}$ .

Then we have:

$$\gamma(\vec{q}) = \gamma - \frac{1}{2N} \sum_{ij} \gamma_{ij} [\vec{q} \cdot (\vec{r}_i - \vec{r}_j)]^2$$

$$\gamma = \sum_j \gamma_{jj}$$

$$\vec{q} \cdot (\vec{r}_i - \vec{r}_j) = \sum_k q_k (\vec{r}_i - \vec{r}_j)_k$$

$$\sum_{ij} \gamma_{ij} [\vec{q} \cdot (\vec{r}_i - \vec{r}_j)]^2 =$$

$$= \sum_{ij} \gamma_{ij} \sum_{\lambda \lambda'} q_\lambda q_{\lambda'} (\vec{r}_i - \vec{r}_j)_\lambda (\vec{r}_i - \vec{r}_j)_{\lambda'} = *$$

Due to inversion symmetry we have:

$$* = \sum_{ij} \gamma_{ij} \sum_\lambda q_\lambda^2 (\vec{r}_i - \vec{r}_j)_\lambda^2 =$$

$$= \frac{1}{d} \sum_{ij} \gamma_{ij} |\vec{r}_i - \vec{r}_j|^2 q^2$$

where  $d$  is the ~~lattice~~ lattice dimension.

$$\text{let } K = \frac{1}{Nd} \sum_{ij} \gamma_{ij} |\vec{r}_i - \vec{r}_j|^2$$

Then we have:

$$\mathcal{I}(\vec{q}) \approx \mathcal{I} - \frac{1}{2} K q^2$$

$$G(\vec{q}) = \frac{1}{1 - \frac{1}{T} (\mathcal{I} - \frac{1}{2} K q^2)} =$$

$$= \frac{1}{1 - \frac{\mathcal{I}}{T} + \frac{1}{2T} K q^2}$$

Recall that  $T_c = \mathcal{I}$  in MFT.

Then we have:

$$G(\vec{q}) = \frac{T}{T - T_c + \frac{1}{2} K q^2}$$

~~state occupation~~

what does this correspond to in real space?

$$f(\vec{r}) = \frac{1}{N} \sum_{\vec{q}} G(\vec{q}) e^{i \vec{q} \cdot \vec{r}}$$

Calculate for ~~the~~  $d=3$  for concreteness.

$$\sum_{\vec{q}} \rightarrow \frac{V^3}{(2\pi)^3} \int d\vec{q}$$

$$\frac{V^3}{N} = a^3$$

$$G(r) = a^3 \int \frac{d\vec{q}}{(2\pi)^3} f(\vec{q}) e^{i\vec{q} \cdot \vec{r}} =$$

$$= \frac{a^3}{8\pi^3} \int_0^\infty dq \int_0^\pi d\theta \sin\theta \int_0^\alpha dq \cdot q^2 f(\vec{q}) e^{i(qr - q\cos\theta)} =$$

$$= \frac{a^3}{\pi^2 r} \int_0^\alpha dq \cdot q^2 \frac{\sin qr}{qr} f(\vec{q}) =$$

$$= \frac{a^3 T}{\pi^2 r K} \int_0^\alpha dq \cdot q \frac{\sin (qr)}{T - T_c + \frac{1}{2} K q^2} =$$

$$= \frac{a^3 T}{\pi^2 r K} \int_0^\alpha \frac{dq \cdot q \cdot \sin (qr)}{\left( q - i\sqrt{2 \frac{T-T_c}{K}} \right) \left( q + i\sqrt{2 \frac{T-T_c}{K}} \right)} =$$

$$= \frac{a^3 T}{\pi^2 r K} \frac{1}{2} \cdot \frac{1}{\pi} \int_{-\infty}^\infty dq \cdot q \frac{e^{iqr} - e^{-iqr}}{\left( q - i\sqrt{2 \frac{T-T_c}{K}} \right) \left( q + i\sqrt{2 \frac{T-T_c}{K}} \right)} =$$

$$= 2 \cdot \frac{a^3 T}{4\pi^2 i \tau K} \left( \sqrt{2} \frac{T-T_c}{K} - \frac{1}{2i\sqrt{2} \frac{T-T_c}{K}} e^{-\sqrt{2} \frac{T-T_c}{K} \cdot r} \right) =$$

$$= \frac{a^3 T}{2\pi K r} e^{-\sqrt{2} \frac{T-T_c}{K} r}$$

Introduce correlation length:

$$\xi = \sqrt{\frac{K}{2(T-T_c)}}$$

$$G(r) \sim \frac{e^{-r/\xi}}{r}$$

$$\text{generally: } G(r) \sim \frac{e^{-r/\xi}}{r^{d-2}}$$

$$\xi \sim (T-T_c)^{-\nu}$$

$\nu = \frac{1}{2}$  - mean-field correlation length exponent.

$\xi$  diverges as  $T$  approaches  $T_c$ , either from below or from above.