

Lecture 3

In lecture 2 we started proving the gaussian integral identity:

$$\frac{1}{(2\pi)^{N/2}} \int_{-\infty}^{\infty} dy_1 \dots dy_N e^{-\frac{1}{2} \varphi_i A_{ij} \varphi_j + \varphi_i \delta_i} =$$

$$= \frac{1}{\sqrt{\det A}} e^{\frac{1}{2} \delta_i A^{-1}_{ij} \delta_j}$$

This is just ~~the~~ the N -dimensional generalization of the gaussian integral:

$$\int_{-\infty}^{\infty} dx e^{-\frac{1}{2} \alpha x^2 + bx} = \sqrt{\frac{2\pi}{\alpha}} e^{\frac{1}{2} \frac{b^2}{\alpha}}$$

Prove by completing the square:

$$y_i = \varphi_i - A^{-1}_{ij} \delta_j$$

and then diagonalizing the matrix A :

$$z_i = U^{-1}_{ij} y_j$$

Then we obtain:

$$\frac{1}{(2\pi)^{N/2}} \int_{-\infty}^{\infty} d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2} \sum_i \varphi_i A_{ij} \varphi_j + \sum_i \varphi_i \delta_i} = \\ = \frac{1}{(2\pi)^{N/2}} \int_{-\infty}^{\infty} dz_1 \dots dz_N e^{-\frac{1}{2} \sum_i \lambda_i z_i^2 + \frac{1}{2} \sum_i \delta_i A_{ij}^{-1} \delta_j} =^*$$

Here we have used the fact that the Jacobian of the transformation from φ to z variables is equal to 1 ($= \det U$).

λ_i are eigenvalues of A , $\lambda_i > 0$.

Then $\int_{-\infty}^{\infty} dz_i e^{-\frac{1}{2} \lambda_i z_i^2} = \sqrt{\frac{2\pi}{\lambda_i}}$

$$^* = \frac{1}{(2\pi)^{N/2}} \prod_{i=1}^N \sqrt{\frac{2\pi}{\lambda_i}} e^{\frac{1}{2} \sum_i \delta_i A_{ij}^{-1} \delta_j} = \\ = \frac{1}{\sqrt{\det A}} e^{\frac{1}{2} \sum_i \delta_i A_{ij}^{-1} \delta_j}$$

Let's apply this identity to the partition function of the Ising model:

$$e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j} = (\det y^{-1})^{1/2} T^{N/2} \frac{1}{(2\pi)^{N/2}} \cdot \\ \int_{-\infty}^{\infty} d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2} \sum_{ij} \varphi_i y_{ij}^{-1} \varphi_j + \sum_i \varphi_i \delta_i}$$

It's convenient to change the integration variables:

$$\varphi_i \rightarrow \frac{\varphi_i}{T}$$

Then we have:

$$\begin{aligned} Z &= \sum_{\{\sigma\}} e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j} = \\ &= C \sum_{\{\sigma\}} \int_{-\infty}^{\infty} d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2T} \sum_{ij} \cancel{\varphi_i J_{ij}^{-1} \varphi_j}} \\ &\cdot e^{\frac{1}{T} \sum_i \varphi_i \sigma_i} \end{aligned}$$

$$\text{Here } C = (\det J)^{-\frac{1}{2}} (2\pi T)^{-\frac{N}{2}}$$

J is an $N \times N$ matrix with matrix elements J_{ij} .

C is a constant that doesn't affect any physical thermodynamic properties \Rightarrow we will ignore it henceforth.

$$\begin{aligned} Z &= \sum_{\{\sigma\}} e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j} = \\ &= \sum_{\{\varphi\}} \int_{-\infty}^{\infty} d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2T} \sum_{ij} \varphi_i J_{ij}^{-1} \varphi_j + \frac{1}{T} \sum_i \varphi_i \sigma_i} \end{aligned}$$

Thus we have transformed the partition function of a system of interacting spins σ_i into partition function of independent spins interacting with a fluctuating "magnetic field" φ_i . The physical meaning of φ_i is Fluctuating molecular field.

To see this compare with the ~~partition~~ mean-field partition function of the Ising model:

$$Z = \sum_{\{ \sigma \}} e^{-\frac{1}{2T} N \gamma M^2 + \frac{1}{T} M \gamma \sigma_i}$$

$B_m = M \gamma$ - molecular field.

$$Z = \sum_{\{ \sigma \}} e^{-\frac{1}{2T} N \gamma^{-1} B_m^2 + \frac{1}{T} B_m \sigma_i}$$

Thus φ_i is a fluctuating position-dependent molecular field.

This transformation of the partition function is called Hubbard-Stratonovich transformation.

Since the spin variables are decoupled we can calculate the sum over spin configurations, just as we did in mean-field theory:

$$Z = \sum_{\{q\}} \int d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2T} \sum_{ij} \varphi_i J_{ij}^{-1} \varphi_j}$$

$$e^{\frac{1}{T} \sum_i \varphi_i \sigma_i}$$

Introduce short-hand notation:

$$D\varphi = d\varphi_1 \dots d\varphi_N$$

$$Z = \int D\varphi e^{-\frac{1}{2T} \sum_{ij} \varphi_i J_{ij}^{-1} \varphi_j + \sum_i \ln[2 \cosh(\frac{\varphi_i}{T})]}$$

Introduce functional:

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

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

We have transformed the problem of calculating the partition function of the Ising model to the problem of calculating a multidimensional integral of an exponential.

Mean-field theory corresponds to an approximate evaluation of this integral using ~~the~~ the saddle-point method.

In this case we have:

$$Z = \int D\varphi e^{-S[\varphi]} \approx \boxed{\dots} e^{-S[\bar{\varphi}]}$$

where $\bar{\varphi} = (\bar{\varphi}_1, \dots, \bar{\varphi}_n)$ is the configuration of ~~the~~ variables φ_i that minimizes $S[\varphi]$.

~~We can expect in the case of the Ising model that~~

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

Minimizing $S[\varphi]$, we obtain:

$$\frac{1}{T} \sum_j J_{ij}^{-1} \bar{\varphi}_j - \frac{1}{T} \tanh\left(\frac{\bar{\varphi}_i}{T}\right) = 0.$$

~~Multiplying both sides by J (matrix multiplication), we obtain:~~

$$\bar{\varphi}_i = \sum_j J_{ij} \tanh\left(\frac{\bar{\varphi}}{T}\right)$$

~~Due to translational invariance the solution will be independent of site index i :~~

$$\bar{\varphi} = \sum_j J_{ij} \tanh\left(\frac{\bar{\varphi}}{T}\right)$$

$$\bar{\varphi} = \boxed{\dots} J \tanh\left(\frac{\bar{\varphi}}{T}\right)$$

This is nothing but the mean-field equation for molecular field B_m , i.e. $\bar{\varphi} = B_m$ as expected.

Now the rigorous meaning of mean-field theory is that it corresponds to saddle-point approximation to the functional integral representation of the partition function of the Ising model:

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

Let's prove that mean-field approximation is exact for the infinite-range Ising model.

Let $J_{ij} = \frac{J}{N}$ - between any two sites.

$$\sum_j J_{ij} = J$$

$$\begin{aligned} \mathcal{H} &= -\frac{1}{2} \sum_{ij} J_{ij} \sigma_i \sigma_j = -\frac{J}{2N} \sum_{ij} \sigma_i \sigma_j = \\ &= -\frac{J}{2N} \left(\sum_i \sigma_i \right)^2 \end{aligned}$$

The Hubbard-Stratonovich transformation only requires one field:

$$e^{\frac{J}{2NT} \left(\sum_i \sigma_i \right)^2} = \int_{-\infty}^{\infty} d\varphi e^{-\frac{N}{2JT} \varphi^2 + \frac{\varphi}{T} \sum_i \sigma_i}$$

The partition function becomes:

$$Z = \sum_{\{o_i\}} \int d\varphi e^{-\frac{N}{2kT}\varphi^2 + \frac{\varphi}{T} \sum_i o_i} =$$

$$= \int d\varphi e^{-\frac{N}{2kT}\varphi^2 + \sum_i \ln[2\cosh(\frac{\varphi}{T})]} =$$

~~$\int d\varphi e^{-\frac{N}{2kT}\varphi^2 + N \ln[2\cosh(\frac{\varphi}{T})]}$~~

$$= \int d\varphi e^{-\frac{N}{2kT}\varphi^2 + N \ln[2\cosh(\frac{\varphi}{T})]}$$

Define $S[\varphi] = \frac{1}{2kT}\varphi^2 - \ln[2\cosh(\frac{\varphi}{T})]$

$$Z = \int d\varphi e^{-NS[\varphi]}$$

Let $\bar{\varphi}$ be the value of ~~φ~~ φ that minimizes S .

$$\bar{\varphi} = T \tanh\left(\frac{\bar{\varphi}}{T}\right)$$

Expand $S[\varphi]$ in Taylor series around $\bar{\varphi}$.

$$S[\varphi] \approx S[\bar{\varphi}] + \frac{1}{2} \frac{d^2 S}{d\varphi^2} \delta\varphi^2 + \dots$$

$$\delta\varphi = \varphi - \bar{\varphi}$$

$\frac{d^2S}{d\varphi^2} > 0$ since $\bar{\varphi}$ is a minimum.

Then we obtain:

$$Z = \int d\varphi e^{-NS[\varphi]} = e^{-NS[\bar{\varphi}]}$$

$$\begin{aligned} \cdot \int d\delta\varphi e^{-\frac{N}{2} \frac{d^2S}{d\varphi^2}} \Big|_{\varphi=\bar{\varphi}} \delta\varphi^2 &= \\ &= e^{-NS[\bar{\varphi}]} \sqrt{\frac{2\pi}{N \frac{d^2S}{d\varphi^2}}} \end{aligned}$$

Calculate the free energy:

$$F = -T \ln Z = TN S[\bar{\varphi}] - \frac{1}{2} \ln \left(\frac{1}{N} N \frac{d^2S}{d\varphi^2} \right)$$

As $N \rightarrow \infty$, $\ln N$ becomes negligible compared to N .

thus $F = TN S[\bar{\varphi}] - MFT$ is exact.

Thus another way to think about MFT is that this is an approximation that becomes exact in the limit of infinite-range interaction.

Introduce spin-spin correlation function.

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

B_i - site-dependent magnetic field, we need it only as a mathematical device.

Define spin-spin correlation function as:

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

Let's show that G_{ij} for $\mathcal{H} = -\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j$ can be calculated as:

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

$$F = -T \ln Z$$

$$\frac{\partial^2 F}{\partial B_i \partial B_j} = -T \left. \frac{\partial^2}{\partial B_i \partial B_j} (\ln Z) \right. =$$

$$= -T \frac{\partial}{\partial B_j} \left(\frac{1}{Z} \frac{\partial Z}{\partial B_i} \right) =$$

$$= -T \frac{1}{Z} \frac{\partial^2 Z}{\partial B_i \partial B_j} + T \frac{1}{Z^2} \left(\frac{\partial Z}{\partial B_i} \right) \left(\frac{\partial Z}{\partial B_j} \right)$$

$$Z = \sum_{\{\sigma_i\}} e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j + \frac{1}{T} \sum_i B_i \sigma_i}$$

$$\left. \frac{\partial Z}{\partial B_i} \right|_{B=0} = \sum_{\{\sigma_i\}} \frac{1}{T} \sigma_i e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j}$$

Thus $\frac{T}{Z} \left. \frac{\partial Z}{\partial B_i} \right|_{B=0} = \langle \sigma_i \rangle$

$$\left. \frac{\partial^2 Z}{\partial B_i \partial B_j} \right|_{B=0} = \sum_{\{\sigma_i\}} \frac{\sigma_i \sigma_j}{T^2} e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j}$$

Thus $\langle \sigma_i \sigma_j \rangle = \frac{T^2}{Z} \left. \frac{\partial^2 Z}{\partial B_i \partial B_j} \right|_{B=0}$

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

Now consider functional integral representation of the Ising model.

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

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

Calculate G_{ij}

$$\begin{aligned} G_{ij} &= -T \left. \frac{\partial^2 F}{\partial B_i \partial B_j} \right|_{B=0} = \\ &= T^2 \frac{1}{Z} \left. \frac{\partial^2 Z}{\partial B_i \partial B_j} \right|_{B=0} - T^2 \frac{1}{Z^2} \left. \frac{\partial Z}{\partial B_i} \right|_{B=0} \left. \frac{\partial Z}{\partial B_j} \right|_{B=0} \end{aligned}$$

change integration variable in the functional integral:

$$\varphi_i \rightarrow \varphi_i - B_i$$

Then we obtain:

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

Then we have:

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

~~oooooooooooo~~ change variables again:

$$\text{let } m_i = \sum_j \tilde{J}_{ij}^{-1} \varphi_j$$

The physical meaning of m_i is fluctuating magnetization at site i .

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

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

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

Analogously :

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

Now :

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

let us now calculate G_{ij} in the mean-field approx.

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

m minimizes S .

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

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

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

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

$$\begin{aligned} g_{ij} &= -T \frac{\partial^2 F}{\partial B_i \partial B_j} \Big|_{B=0} = T \frac{\partial m_i}{\partial B_j} \Big|_{B=0} = \\ &= T \frac{\partial}{\partial B_j} \tanh \left(\frac{\sum_e J_{ie} m_e + B_i}{T} \right) = \\ &= \left[\delta_{ij} + \sum_e J_{ie} \frac{\partial m_e}{\partial B_j} \Big|_{B=0} \right] \left[1 - \tanh^2 \left(\frac{\sum_e J_{ie} m_e}{T} \right) \right] \\ &= \left[\delta_{ij} + \frac{1}{T} \sum_e J_{ie} g_{ej} \right] (1 - m^2) \end{aligned}$$

Thus we set the following equation for g_{ij} :

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

We are interested in the ~~correlation~~ behavior of the correlation function near T_c , where m is small (≈ 0) so m^2 can be neglected.
Thus we finally obtain:

$$\sum_e \left[\delta_{ie} - \frac{1}{T} J_{ie} \right] g_{ej} = \delta_{ij}$$