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# Mean-field approximation and Landau theory

We consider the Hamiltonian:

$$H = \hat{M}_i \lambda_{ij} \hat{M}_j.$$

For repeated indices, we take the sum. We consider a mean-field Hamiltonian given by

$$H(\boldsymbol{M}) = M_i \lambda_{ij} \hat{M}_j + \hat{M}_i \lambda_{ij} M_j - M_i \lambda_{ij} M_j,$$

where $\boldsymbol{M}$ is called an order parameter. We assume that the order parameter transforms in the same way as the operator $\hat{\boldsymbol{M}}$ under symmetry operations. Then the mean-field Hamiltonian has the same symmetry as the original Hamiltonian. The original and mean-field Hamiltonians have the following relationship:

$$H = H(\boldsymbol{M}) + (\hat{M}_i - M_i)\lambda_{ij}(\hat{M}_j - M_j).$$

In the mean-field approximation, we ignore the fluctuations given by the last term in this equation. In the non-ordered state with $\boldsymbol{M} = \boldsymbol{0}$ or the critical region with small $\boldsymbol{M}$ around the transition point, the non-fluctuation terms are zero or very small and the mean-field approximation is not justified. In the mean-field approximation, we assume that $\boldsymbol{M}$ is equal to the expectation value of $\hat{\boldsymbol{M}}$ in the mean-filed Hamiltonian:

$$\boldsymbol{M} = \langle \hat{\boldsymbol{M}} \rangle_{\mathrm{MF}} = \frac{\mathrm{Tr} \hat{\boldsymbol{M}} e^{-\beta H(\boldsymbol{M})}}{\mathrm{Tr} e^{-\beta H(\boldsymbol{M})}}.$$

It is called a mean-field equation.

We consider the free energy of the mean-field Hamiltonian:

$$F(\boldsymbol{M}) = -\frac{1}{\beta} \ln \mathrm{Tr} e^{-\beta H(\boldsymbol{M})}.$$

By using

$$\begin{aligned}
\frac{\partial H(\boldsymbol{M})}{\partial M_i} &= \lambda_{ij} \hat{M}_j + \hat{M}_j \lambda_{ji} - \lambda_{ij} M_j - M_j \lambda_{ji} \\
&= \lambda_{ij}(\hat{M}_j - M_j) + (\hat{M}_j - M_j)\lambda_{ji} \\
&= (\lambda_{ij} + \lambda_{ji})(\hat{M}_j - M_j),
\end{aligned}$$

the derivative of $F(\boldsymbol{M})$ with respect to $M_i$ is

$$\frac{\partial F(\boldsymbol{M})}{\partial M_i} = \frac{\mathrm{Tr}\frac{\partial H(\boldsymbol{M})}{\partial M_i} e^{-\beta H(\boldsymbol{M})}}{\mathrm{Tr} e^{-\beta H(\boldsymbol{M})}} = (\lambda_{ij} + \lambda_{ji})(\langle \hat{M}_j \rangle_{\mathrm{MF}} - M_j).$$

Therefore the condition that $F(\boldsymbol{M})$ is an extremum is equivalent to the mean-field equation. However, only from the above discussion, we cannot determine which solution we should choose when there are multiple solutions.

Then, we assume $\langle H(\boldsymbol{M}) \rangle_{\mathrm{MF}} = \langle H \rangle_{\mathrm{MF}}$ when the mean-field equation holds. In this case, we should choose the solution with the lowest free energy based on the Bogoliubov-Feynman inequality (cf. calculation memo "Variational principle for free energy"). From this discussion, we can use $F(\boldsymbol{M})$ as the free energy of the Landau theory and we should minimize this.

In the actual calculation of mean-field approximation, it is usually easier to solve the mean-field equation than to minimize the free energy and the following procedure is often applied:

1. Choose a mean-field Hamiltonian that satisfies $\langle H(\boldsymbol{M}) \rangle_{\mathrm{MF}} = \langle H \rangle_{\mathrm{MF}}$ when the mean-field equation holds.

2. Solve the mean-field equation.

3. Select the solution with the lowest free energy.

## Mean-field approximation for the Ising model

We consider the following Hamiltonian:

$$H = -J \sum_{<i,j>} \hat{M}_i \hat{M}_j,$$

where $\hat{M}_i = \pm 1$, $i$ and $j$ represent lattice sites, $<i,j>$ denotes summation over pairs of nearest-neighboring sites. We consider an order parameter $M$ independent of the site. Then, the mean-field Hamiltonian is given by

$$\begin{aligned} H(M) &= -J \sum_{<i,j>} \left( M\hat{M}_j + \hat{M}_i M - M^2 \right) \\ &= -J \sum_{<i,j>} \left( 2M\hat{M}_i - M^2 \right) \\ &= -J \sum_{i} \frac{z}{2} \left( 2M\hat{M}_i - M^2 \right) \\ &= N\frac{z}{2} JM^2 - zJM \sum_{i} \hat{M}_i. \end{aligned}$$

Here, $z$ is the number of nearest-neighboring lattice sites and $N$ is the total number of the lattice sites. In this mean-field Hamiltonian, we can sum the states at each site independently and then, $\langle \hat{M}_i \hat{M}_j \rangle_{\rm MF} = \langle \hat{M}_i \rangle_{\rm MF} \langle \hat{M}_j \rangle_{\rm MF}$. In addition, if the mean-field equation $\langle \hat{M}_i \rangle_{\rm MF} = M$ holds, we obtain $\langle H(M) \rangle_{\rm MF} = \langle H \rangle_{\rm MF}$.

$$\langle \hat{M}_i \rangle_{\rm MF} = \frac{e^{\beta zJM} - e^{-\beta zJM}}{e^{\beta zJM} + e^{-\beta zJM}} = \tanh(\beta zJM).$$

Then, the mean-field equation is $M = \tanh(\beta zJM)$. For $J \leq 0$, there is only one solution $M = 0$. In the following, we assume $J > 0$. For $0 \leq M \ll 1$,

$$M = \tanh(\beta zJM) \simeq \beta zJM - \frac{1}{3}(\beta zJ)^3 M^3.$$

From the coefficients of 1st-order terms of $M$, a solution with non-zero $M$ appears for $T < T_{\rm c} = zJ$. By using this, we can rewrite the above equation as

$$\left( \frac{T_{\rm c}}{T} - 1 \right) M \simeq \frac{1}{3} \left( \frac{T_{\rm c}}{T} \right)^3 M^3.$$

Then, for $T \lesssim T_{\rm c}$, we obtain a solution with non-zero $M$:

$$M \simeq \sqrt{3(T_{\rm c} - T)/T_{\rm c}}.$$

However, we cannot determine which solution, $M = 0$ or $M \neq 0$, should we choose only from this calculation.

## Landau theory for the Ising model

$$\begin{aligned}
{\rm Tr} e^{-\beta H(M)} &= {\rm Tr} e^{-\beta \left( N \frac{T_{\rm c}}{2} M^2 - T_{\rm c} M \sum_i \hat{M}_i \right)} \\
&= e^{-\beta N \frac{T_{\rm c}}{2} M^2} {\rm Tr} e^{\beta T_{\rm c} M \sum_i \hat{M}_i} \\
&= e^{-\beta N \frac{T_{\rm c}}{2} M^2} {\rm Tr} \prod_i e^{\beta T_{\rm c} M \hat{M}_i} \\
&= e^{-\beta N \frac{T_{\rm c}}{2} M^2} \left( e^{\beta T_{\rm c} M} + e^{-\beta T_{\rm c} M} \right)^N .
\end{aligned}$$

We expand the free energy up to 4th order in $M$. By using

$$\begin{aligned}
\ln(e^x + e^{-x}) &= \ln\left[\left(1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + \cdots\right) + \left(1 - x + \frac{x^2}{2} - \frac{x^3}{6} + \frac{x^4}{24} + \cdots\right)\right] \\
&= \ln\left[2\left(1 + \frac{x^2}{2} + \frac{x^4}{24} + \cdots\right)\right] \\
&= \ln 2 + \ln\left(1 + \frac{x^2}{2} + \frac{x^4}{24} + \cdots\right) \\
&= \ln 2 + \left(\frac{x^2}{2} + \frac{x^4}{24} + \cdots\right) - \frac{1}{2}\left(\frac{x^2}{2} + \frac{x^4}{24} + \cdots\right)^2 + \cdots \\
&\simeq \ln 2 + \frac{x^2}{2} - \frac{x^4}{12},
\end{aligned}$$

$$\begin{aligned}
F(M) = -T \ln \mathrm{Tr} e^{-\beta H(M)} &= N\frac{T_\mathrm{c}}{2}M^2 - NT \ln\left(e^{\beta T_\mathrm{c} M} + e^{-\beta T_\mathrm{c} M}\right) \\
&\simeq N\frac{T_\mathrm{c}}{2}M^2 - NT\ln 2 - NT\frac{1}{2}\left(\frac{T_\mathrm{c}}{T}\right)^2 M^2 + NT\frac{1}{12}\left(\frac{T_\mathrm{c}}{T}\right)^4 M^4 \\
&= -NT\ln 2 + N\left[-\frac{T_\mathrm{c}}{2}\left(\frac{T_\mathrm{c}}{T} - 1\right)M^2 + \frac{T_\mathrm{c}}{12}\left(\frac{T_\mathrm{c}}{T}\right)^3 M^4\right].
\end{aligned}$$

$$\frac{dF(M)}{dM} \simeq NMT_\mathrm{c}\left[-\left(\frac{T_\mathrm{c}}{T} - 1\right) + \frac{1}{3}\left(\frac{T_\mathrm{c}}{T}\right)^3 M^2\right].$$

Thus, for $T \lesssim T_\mathrm{c}$, we obtain a non-zero $M$ solution of $dF(M)/dM = 0$,

$$M \simeq \sqrt{3(T_\mathrm{c} - T)/T_\mathrm{c}},$$

as obtained by solving the mean-field equation directly. In addition, we find that the above solution $M \neq 0$ minimizes $F(M)$ since the coefficient of $M^2$ in $F(M)$ is negative at $T \lesssim T_\mathrm{c}$.

Even without expanding $F(M)$, we can easily show that the condition that $F(M)$ is an extremum is equivalent to the mean-field equation:

$$\begin{aligned}
\frac{dF(M)}{dM} &= NT_\mathrm{c}M - NT\beta T_\mathrm{c}\frac{e^{\beta T_\mathrm{c} M} - e^{-\beta T_\mathrm{c} M}}{e^{\beta T_\mathrm{c} M} + e^{-\beta T_\mathrm{c} M}} \\
&= NT_\mathrm{c}\left[M - \tanh\left(\frac{T_\mathrm{c}}{T}M\right)\right].
\end{aligned}$$