Approximating the Ising model [tln97]

Quite generally, approximations ignore at least some of the correlations between microscopic degrees of freedom.

Correlated fluctuations tend to be stronger in low dimensions. Hence their neglect has milder consequences in high dimensions.

Mean-field approximation:

Ising model Hamiltonian: $\mathcal{H} = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - H\sum_i \sigma_i$.

The mean-field approximation ignores all spin correlations: $\langle\sigma_i\sigma_j\rangle \to \langle\sigma_i\rangle\langle\sigma_j\rangle$.

The Ising interaction term is thus effectively reduced to a (mean-field) contribution to the external magnetic field:

$$\mathcal{H}_{\rm MF} = -H_{\rm eff}\sum_{i=1}^{N}\sigma_i, \quad H_{\rm eff} = H + zJ\langle\sigma_j\rangle = H + zJ\bar{M}.$$

The coordination number z counts the number of nearest neighbors to site j on the lattice (assumed to be uniform).

The partition function of $\mathcal{H}_{\rm MF}$ is formally equivalent to that of two-level paramagnet [tex85] and the Gibbs free energy follows directly:

$$Z_{\rm MF} = \big[2\cosh(\beta H_{\rm eff})\big]^N \quad \Rightarrow \; G(T,H,N) = -Nk_BT\ln\big(2\cosh(\beta H_{\rm eff})\big).$$

The magnetization (per site) is a first partial derivative and produces the mean-field equation of state analyzed in [tln84]:

$$\bar{M} = -\frac{1}{N}\frac{\partial G}{\partial H} = \tanh\big(\beta(H + zJ\bar{M})\big).$$

Bragg-Williams approximation:

Here a different chain of reasoning leads to the same result.

Canonical partition function, density operator, and Gibbs free energy:

$$Z = {\rm Tr}[\rho], \quad \rho = e^{-\beta\mathcal{H}}, \quad G = -k_BT\ln Z.$$

Factorization assumption and uniformity:

$$\rho = \prod_{i=1}^{N}\rho_i, \quad \rho_i = \begin{pmatrix} \frac{1+m_i}{2} & 0 \\ 0 & \frac{1-m_i}{2}\end{pmatrix}, \quad m_i = \langle\sigma_i\rangle = \bar{M}.$$

Enthalpy: $E[\bar{M}] \doteq \mathrm{Tr}[\rho\mathcal{H}] = \frac{1}{2}NzJ\bar{M}^2 - NH\bar{M}$.

Entropy: $S[\bar{M}] \doteq -k_B\mathrm{Tr}[\rho\ln\rho] = -Nk_B\left[\frac{1+\bar{M}}{2}\ln\frac{1+\bar{M}}{2} + \frac{1-\bar{M}}{2}\ln\frac{1-\bar{M}}{2}\right]$.

Gibbs free energy functional: $G[\bar{M}] = E[\bar{M}] - TS[\bar{M}]$.

Order parameter from extremum principle: $\frac{dG}{d\bar{M}} = 0$.

$$\Rightarrow \quad -zJ\bar{M} - H + k_BT\underbrace{\frac{1}{2}\ln\left(\frac{1+\bar{M}}{1-\bar{M}}\right)}_{\mathrm{Artanh}\bar{M}} = 0.$$

Mean-field equation of state follows: $\bar{M} = \tanh\big(\beta(H + zJ\bar{M})\big)$.

Bethe approximation:

The Bethe approximation is one step above the mean-field approximation. It rigorously accounts for pair correlations between nearest-neighbor spin.

Consider a cluster consisting of a central site 0 surrounded by z nearest-neighbor sites j. The cluster Hamiltonian reads,

$$\mathcal{H}_\mathrm{c} = -J\sum_{j=1}^{z}\sigma_0\sigma_j - H\sigma_0 - H'\sum_{j=1}^{z}\sigma_j.$$

The external magnetic field H couples to the central spin, whereas the surrounding spins couple to a modified field H' to be determined self-consistently.

Canonical cluster partition function:

$$\begin{aligned}
Z_\mathrm{c} &= \sum_{\sigma_0=\pm}\sum_{\{\sigma_j=\pm\}}\exp\left(\beta\left[J\sum_{j=1}^{z}\sigma_0\sigma_j + H\sigma_0 + H'\sum_{j=1}^{z}\sigma_j\right]\right)\\
&= e^{\beta H}\sum_{\{\sigma_j=\pm\}}\exp\left((H'+J)\sum_{j=1}^{z}\sigma_j\right) + e^{-\beta H}\sum_{\{\sigma_j=\pm\}}\exp\left((H'-J)\sum_{j=1}^{z}\sigma_j\right)\\
&= e^{\beta H}\Big[2\cosh\big(\beta[J+H']\big)\Big]^z + e^{-\beta H}\Big[2\cosh\big(\beta[J-H']\big)\Big]^z.
\end{aligned}$$

Expectation values for the central cluster spin:

$$\begin{aligned}
\langle\sigma_0\rangle &= \frac{1}{Z_\mathrm{c}}\sum_{\sigma_0=\pm}\sum_{\{\sigma_j=\pm\}}\sigma_0 e^{-\beta\mathcal{H}_\mathrm{c}} = \frac{k_BT}{Z_\mathrm{c}}\frac{\partial Z_\mathrm{c}}{\partial H} = \frac{\partial}{\partial H}\Big(k_BT\ln Z_c\Big)\\
&= \frac{1}{Z_\mathrm{c}}\left\{e^{\beta H}\Big[2\cosh\big(\beta[J+H']\big)\Big]^z - e^{-\beta H}\Big[2\cosh\big(\beta[J-H']\big)\Big]^z\right\}.
\end{aligned}$$

Expectation values for the surrounding cluster spin:

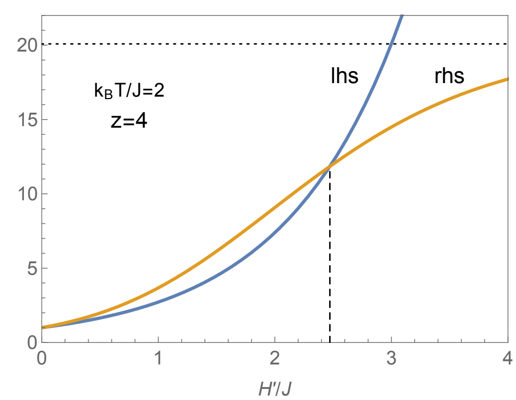
$$\langle\sigma_j\rangle = \frac{1}{Z_\mathrm{c}}\sum_{\sigma_0=\pm}\sum_{\{\sigma_j=\pm\}}\sigma_j e^{-\beta\mathcal{H}_\mathrm{c}} = \frac{k_BT}{zZ_\mathrm{c}}\frac{\partial Z_\mathrm{c}}{\partial H'} = \frac{1}{z}\frac{\partial}{\partial H'}\Big(k_BT\ln Z_c\Big)$$
$$= \frac{1}{Z_\mathrm{c}}\Big\{e^{\beta H}2\sinh\big(\beta[J+H']\big)\Big[2\cosh\big(\beta[J+H']\big)\Big]^{z-1}$$
$$-e^{-\beta H}2\sinh\big(\beta[J-H']\big)\Big[2\cosh\big(\beta[J-H']\big)\Big]^{z-1}\Big\}.$$

For the case $H=0$, translational invariance, $\langle\sigma_0\rangle = \langle\sigma_j\rangle$, requires that the following relation holds between the dimensionless variables βJ and H'/J:

$$e^{2\beta H'} = \Big[\cosh\big(\beta[J+H']\big)\Big]^{z-1}\Big[\cosh\big(\beta[J-H']\big)\Big]^{1-z}. \tag{1}$$

The solution $H'=0$ always exists and represents $\langle\sigma_0\rangle = \langle\sigma_j\rangle = 0$. A solution $H'>0$, which does not always exist, represents a macrostate with spontaneous ordering, $\langle\sigma_0\rangle = \langle\sigma_j\rangle > 0$ [tex203].

Graphical solutions $H'=0$ and $H'>0$ for a particular case is shown below.

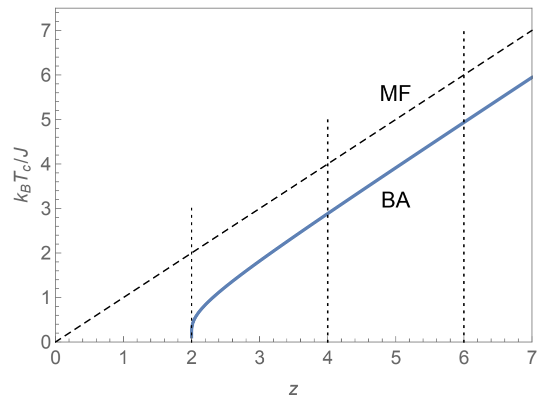


The curve lhs is convex and increases without bound. The curve rhs is monotonic and levels off at $e^{2\beta J(z-1)}$.

The existence of a solution $H'>0$ requires that the initial slope of lhs exceeds the initial slope of rhs. Spontaneous ordering disappears when the two initial slopes are equal.

Critical temperature [tex203]: $(z-1)\tanh\left(\dfrac{J}{k_BT_\mathrm{c}}\right) = 1.$

A plot of k_BT_c/J versus z shows that spontaneous order on a D-dimensional hypercubic lattice, where $z=2D$, does not exist for $D<2$. The mean-field prediction, $k_BT_\mathrm{c}^{(\mathrm{MF})}/J = z$, is shown dashed [tex203].



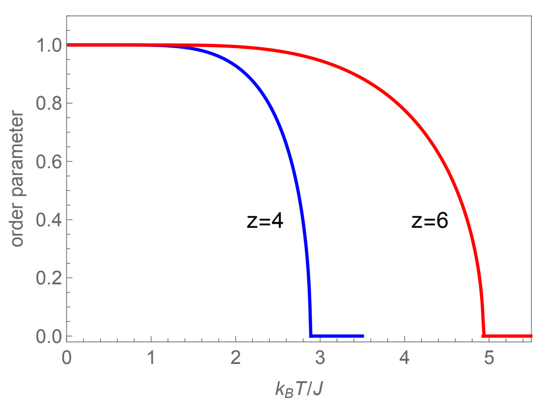
The Bethe approximation overestimates the real transition temperature significantly less than the mean-field approximation does:

$$\frac{T_c}{T_c^{(\mathrm{MF})}} = \begin{cases} 0 & : D = 1, \\ 0.567 & : D = 2, \\ 0.75... & : D = 3, \end{cases} \qquad \frac{T_c}{T_c^{(\mathrm{BA})}} = \begin{cases} 1 & : D = 1, \\ 0.786 & : D = 2, \\ 0.912... & : D = 3. \end{cases}$$

In the limit $D \to \infty$, the three values T_c, $T_c^{(\mathrm{MF})}$, and $T_c^{(\mathrm{BA})}$ converge.

Compiling solutions of (1) with $H' > 0$ for an array of βJ values produces data for the spontaneous magnetization $\langle \sigma_0 \rangle$ (order parameter) [tex203].

The data plotted below show that the Bethe approximation predicts a continuous phase transition in $D = 2$ ($z = 4$) and $D = 3$ ($z = 6$).



Unlike the mean-field approximation, no spontaneous ordering at $T > 0$ is predicted by the Bethe approximation in $D = 1$ ($z = 2$). The partition function predicted by the Bethe approximation for $H' = 0$ is exact:

$$Z_c = 2[\cosh(\beta j)]^2 \quad \Rightarrow \quad Z = \left[\frac{Z_c}{2}\right]^{N/2} = [2\cosh(\beta j)]^N.$$