Modelling of Complex Systems

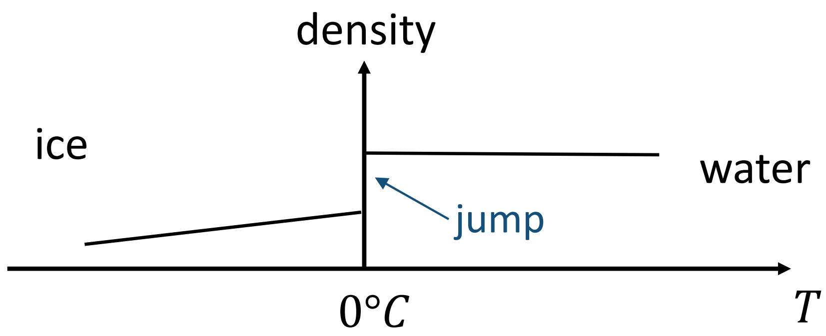
Phase transitions

The one-dimensional Ising model

Phase transitions

By varying the temperature, matter can undergo a transition from one state to another.

For example, the transition ice $\leftrightarrow$ water:



(First-order phase transition)

Symmetry is spontaneously broken at the critical point.

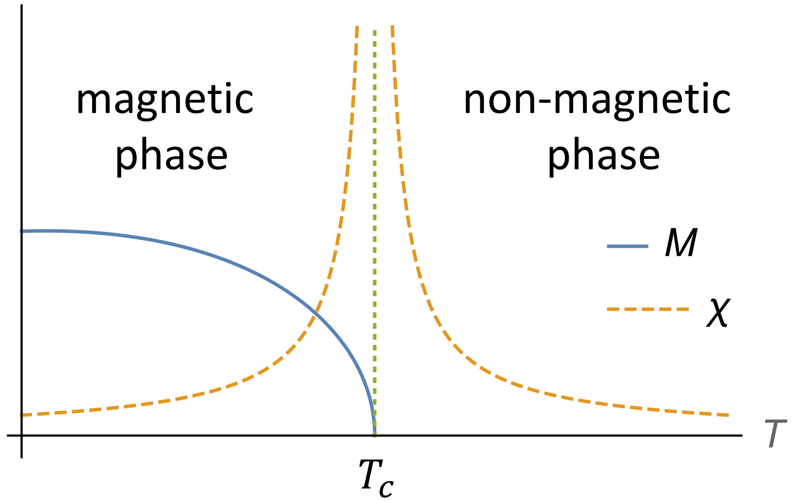
In water: short-range correlations between positions of molecules.
In ice: long-range correlations between positions of molecules. (Molecules are arranged regularly.)

Phase transitions

Magnetic materials

The phase transition from a non-magnetic state (paramagnetic) to a magnetic state (ferromagnetic) is a **continuous transition** (second-order phase transition).

Magnetization M and Susceptibility χ vs. Temperature T



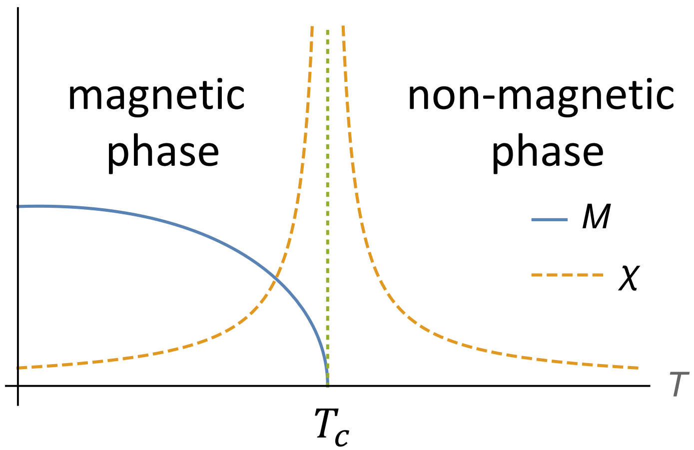
$$\chi \equiv \left.\frac{dM}{dH}\right|_{H=0}$$

Phase transitions

Magnetic materials

- The spontaneous magnetization appears continuously for $T < T_c$:

$$M \propto (T_c - T)^{\beta}, \quad \beta = \begin{cases} 1/8, & 2D \text{ Ising model} \\ \dots & \\ 1/2, & D \geq 4 \end{cases}$$



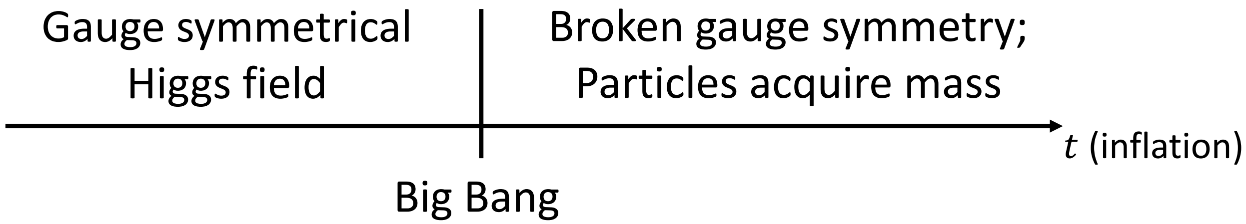
- The magnetic susceptibility (also called response function) diverges at T_c:

$$\chi \equiv \left.\frac{dM}{dH}\right|_{H=0} \propto |T_c - T|^{-\gamma}, \quad \gamma = \begin{cases} 7/4, & 2D \text{ Ising model} \\ \dots & \\ 1, & D \geq 4 \end{cases}$$

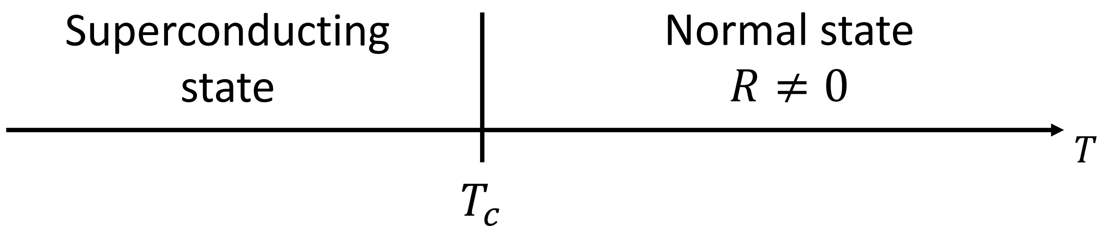
Phase transitions

Other examples of continuous phase transitions:

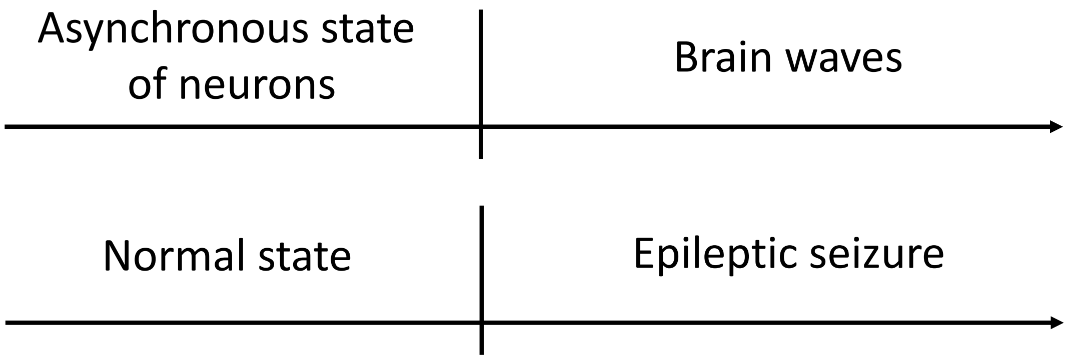
- Standard Model:



- Superconductivity:



- Brain function:

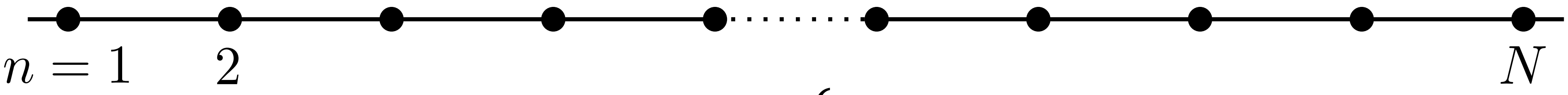


Ising Model

In 1920 Wilhelm Lenz proposed to his PhD student Ernst Ising to solve a magnetic model which we now know as the **Ising model**.

1D Ising model

Consider a one-dimensional lattice (chain) of spins with indices $n = 1, \dots, N$.



Each spin σ_n can take two values: $\sigma_n = \begin{cases} +1, & \text{spin up} \\ -1, & \text{spin down} \end{cases}$.

Neighbouring spins interact with each other:

Energy $= -J\sigma_n\sigma_{n+1} = \begin{cases} -J, & \text{if } \sigma_n = \sigma_{n+1} \text{ (spins are parallel, } \uparrow\uparrow \text{ or } \downarrow\downarrow) \\ J, & \text{if } \sigma_n = -\sigma_{n+1} \text{ (spins are antiparallel } \uparrow\downarrow \text{ or } \downarrow\uparrow) \end{cases}$

The total energy on a ring is $E = -J \sum_{n=1}^{N} \sigma_n \sigma_{n+1}$ where $\sigma_{N+1} \equiv \sigma_1$.

1D Ising Model

In a magnetic field H, each spin contributes with an additional energy from the interaction with the field: energy $= -H\sigma_n = \begin{cases} -H, & \text{if } \sigma_n \text{ parallel to } H \\ H, & \text{if } \sigma_n \text{ antiparallel to } H \end{cases}$

Total energy of the Ising model on a ring in the presence of an external field is:

$$E = -J \sum_{n=1}^{N} \sigma_n \sigma_{n+1} - H \sum_{n=1}^{N} \sigma_n$$

The state of the model is defined by the configuration of spins $(\sigma_1, \sigma_2, \ldots, \sigma_N)$.

The probability of finding the system in a given state $(\sigma_1, \ldots, \sigma_N)$ is

$$w = \frac{1}{Z} \exp\left(-\frac{E(\sigma_1, \ldots, \sigma_N)}{k_B T}\right)$$

Let us we set the Boltzmann constant $k_B = 1$.

1D Ising Model

Normalization: $$\sum_{\{\text{all possible states}\}} w = 1 \implies \sum_{\{\sigma_1=\pm1,\sigma_2=\pm1,\ldots\}} w = 1$$

$$\implies \frac{1}{Z} \sum_{\{\sigma_n=\pm1\}} e^{-E/T} = 1$$

Thus, the **partition function** is defined as $Z \equiv \sum_{\{\sigma_n=\pm1\}} e^{-E/T}$.

The **free energy** is $F = E - TS = -T \ln Z$.

The **total magnetization** is $M = \sum_{n=1}^{N} \sigma_n$.

The **mean magnetic moment** is $m = \frac{1}{N} \sum_{\{\sigma_n=\pm1\}} M(\sigma_1, \ldots, \sigma_N) \frac{e^{-E(\sigma_1,\ldots,\sigma_N)/T}}{Z}$.

1D Ising Model

The mean total magnetization $\langle M \rangle = -\dfrac{\partial F}{\partial H}$:

$$-\frac{\partial F}{\partial H} = \frac{\partial}{\partial H} T \ln Z = \frac{T}{Z}\frac{\partial Z}{\partial H} = \frac{T}{Z}\frac{\partial}{\partial H} \sum_{\{\sigma_n = \pm 1\}} e^{-\beta E}$$

$$= \frac{T}{Z} \sum_{\{\sigma_n = \pm 1\}} \frac{\partial}{\partial H} \exp\left(\beta J \sum_{n=1}^{N} \sigma_n \sigma_{n+1} + \beta H M \right)$$

$$= \frac{T}{Z} \sum_{\{\sigma\}} \beta M e^{-\beta E} = \langle M \rangle$$

where $\beta = 1/T$.

Also, notice the notation $\displaystyle\sum_{\{\sigma\}} \equiv \sum_{\{\sigma_n = \pm 1\}} \equiv \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \cdots \sum_{\sigma_N = \pm 1}$.

1D Ising Model

Let us calculate the partition function by the so-called "transfer matrix method".

For compactness, define $k \equiv J/T$ and $h \equiv H/T$.

Rewrite the partition function as

$$
\begin{aligned}
Z &= \sum_{\{\sigma_n = \pm 1\}} \exp\left(k \sum_{n=1}^{N} \sigma_n \sigma_{n+1} + h \sum_{n=1}^{N} \sigma_n\right) \\
&= \sum_{\{\sigma_n = \pm 1\}} \exp\left(k \sum_{n=1}^{N} \sigma_n \sigma_{n+1} + h \sum_{n=1}^{N} \frac{\sigma_n + \sigma_{n+1}}{2}\right) \\
&= \sum_{\{\sigma_n = \pm 1\}} \prod_{n=1}^{N} \exp\left(k \sigma_n \sigma_{n+1} + h \frac{\sigma_n + \sigma_{n+1}}{2}\right)
\end{aligned}
$$

1D Ising Model

We define a 2-by-2 matrix $\hat{V}$ whose elements are $V_{\sigma\sigma'} = e^{k\sigma\sigma' + \frac{h(\sigma+\sigma')}{2}}$, so that the matrix reads

$$\hat{V} = \begin{bmatrix} V_{1,1} & V_{1,-1} \\ V_{-1,1} & V_{-1,-1} \end{bmatrix} = \begin{bmatrix} e^{k+h} & e^{-k} \\ e^{-k} & e^{k-h} \end{bmatrix}$$

The utility of $\hat{V}$ is that we can write the partition function in terms of this matrix:

$$\begin{aligned} Z &= \sum_{\{\sigma_n = \pm 1\}} \prod_{n=1}^{N} \exp\left(k\sigma_n\sigma_{n+1} + h\frac{\sigma_n + \sigma_{n+1}}{2}\right) \\ &= \sum_{\{\sigma_n = \pm 1\}} V_{\sigma_1,\sigma_2} V_{\sigma_2,\sigma_3} \ldots V_{\sigma_N,\sigma_1} \\ &= \mathrm{Tr}(\hat{V}^N) \end{aligned}$$

1D Ising Model

Matrix $\hat{V}$ is a symmetric real matrix, and, therefore, is diagonalizable.
This means we can represent it in the form $\hat{V} = \hat{P}^{-1}\hat{D}\hat{P}$, where

$$\hat{D} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

is a diagonal matrix whose elements λ_1 and λ_2 are the eigenvalues of $\hat{V}$, and $\hat{P}$ is an orthogonal matrix.

Then, we can write the partition function as

$$\begin{aligned} Z &= \mathrm{Tr}(\hat{V}^N) = \mathrm{Tr}(\hat{P}^{-1}\hat{D}\hat{P}\hat{P}^{-1}\hat{D}\hat{P}...\hat{P}^{-1}\hat{D}\hat{P}) \\ &= \mathrm{Tr}(\hat{P}^{-1}\hat{D}^N\hat{P}) = \mathrm{Tr}(\hat{D}^N) \\ &= {\lambda_1}^N + {\lambda_2}^N \end{aligned}$$

The partition function is determined by the eigenvalues of $\hat{V}$, let us find them.

1D Ising Model

The eigenvalues are solutions of the equation $\det\left|\hat{V} - \lambda\hat{I}\right| = 0$, (where $\hat{I}$ is the identity matrix). That is:

$$\det\begin{vmatrix} e^{k+h}-\lambda & e^{-k} \\ e^{-k} & e^{k-h}-\lambda \end{vmatrix} = 0$$

$$\Rightarrow (e^{k+h}-\lambda)(e^{k-h}-\lambda) - e^{-2k} = 0$$

$$\Leftrightarrow \lambda^2 - \lambda(e^{k+h} + e^{k-h}) + e^{2k} - e^{-2k} = 0$$

$$\Leftrightarrow \lambda^2 - 2\lambda e^k \cosh(h) + e^{2k} - e^{-2k} = 0$$

$$\Leftrightarrow [\lambda - e^k \cosh(h)]^2 - e^{2k}[\cosh^2(h) - 1] - e^{-2k} = 0$$

$$\Leftrightarrow [\lambda - e^k \cosh(h)]^2 - e^{2k}\sinh^2(h) - e^{-2k} = 0$$

$$\Leftrightarrow \lambda = e^k \cosh(h) \pm \sqrt{e^{2k}\sinh^2(h) + e^{-2k}}$$

1D Ising Model

Then, two eigenvalues are:

$$\lambda_1 = e^k \cosh(h) + \sqrt{e^{2k} \sinh^2(h) + e^{-2k}}$$

$$\lambda_2 = e^k \cosh(h) - \sqrt{e^{2k} \sinh^2(h) + e^{-2k}}$$

Notice that $\lambda_1 > \lambda_2$.

Now we can calculate the free energy:

$$F = -T \ln Z = -T \ln({\lambda_1}^N + {\lambda_2}^N)$$

$$= -T \ln \left\{ {\lambda_1}^N \left[1 + \left(\frac{\lambda_2}{\lambda_1} \right)^N \right] \right\}$$

$$= -T \ln {\lambda_1}^N - T \ln \left[1 + \left(\frac{\lambda_2}{\lambda_1} \right)^N \right]$$

1D Ising Model

Recalling that $\lambda_2 < \lambda_1$, we see that $\lim_{N \longrightarrow \infty} \left(\frac{\lambda_2}{\lambda_1}\right)^N = 0$.

Therefore, in the thermodynamic limit, i.e. for $N \longrightarrow \infty$, we have:

$$F = -TN \ln \lambda_1$$

The **free energy per spin** is:

$$f \equiv \frac{F}{N} = -T \ln \lambda_1 = -T \ln \left[e^k \cosh(h) + \sqrt{e^{2k} \sinh^2(h) + e^{-2k}} \right]$$

The **mean magnetic moment** is (recall that $k = \beta J$ and $h = \beta H$):

$$m = -\frac{\partial f}{\partial H} = -\beta \frac{\partial f}{\partial(\beta H)} = -\beta \frac{\partial f}{\partial h}$$

$$= \frac{\partial}{\partial h} \ln \left[e^k \cosh(h) + \sqrt{e^{2k} \sinh^2(h) + e^{-2k}} \right]$$

$$\Rightarrow m = \frac{\sinh h}{\sqrt{\sinh^2 h + e^{-4k}}}$$

1D Ising Model

$$m = \frac{\sinh h}{\sqrt{\sinh^2 h + e^{-4k}}}$$

For **small magnetic field** $h = \frac{H}{T} \ll 1$, the function $\sinh h \cong h$, then

$$m(H,T) \approx \frac{h}{\sqrt{h^2 + e^{-4k}}} = \frac{H}{\sqrt{H + T^2 e^{-4J/T}}} \propto H$$

In the **low-temperature limit**, i.e., when $T \longrightarrow 0$, we have $h = \frac{H}{T} \gg 1$. Then $e^{-4k} \ll \sinh h^2$, and the magnetization is

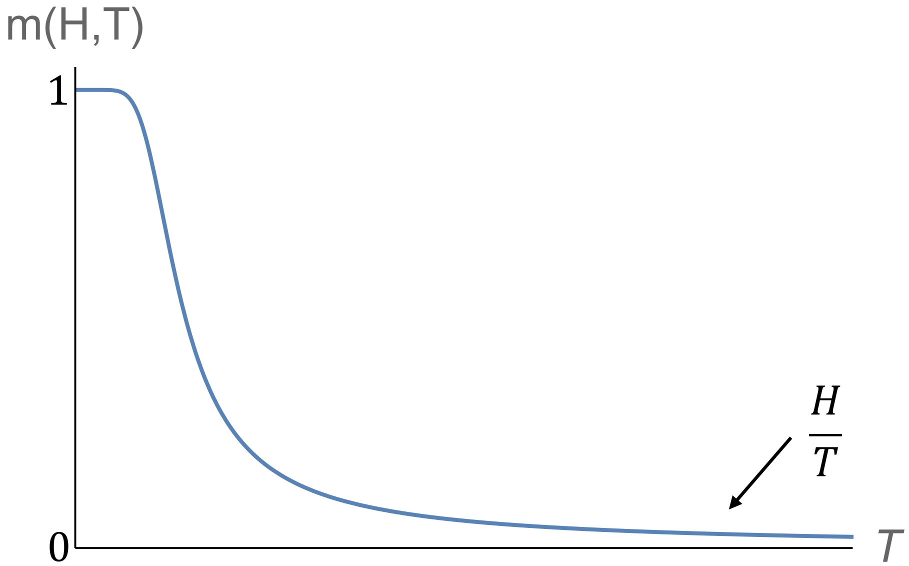
$$m \to \frac{\sinh h}{\sinh h} = 1$$

In the **high-temperature limit**, i.e., when $T \longrightarrow \infty$, we have $k = \frac{J}{T} \ll 1$. Then $e^{-4k} \approx 1$, and the magnetization is

$$m(H,T) \approx \frac{H}{\sqrt{H + T^2}} \approx \frac{H}{T}$$

1D Ising Model

$$m(H,T) = \frac{\sinh(H/T)}{\sqrt{\sinh^2(H/T) + e^{-4J/T}}}$$



Without an external field there is no spontaneous magnetization in the one-dimensional system, i.e., $m(0,T) = 0$. So, there is no phase transition in 1D.

1D Ising Model

The **susceptibility** is $\chi(H,T) = \dfrac{dm}{dH}$.

The zero field ($H = 0$) susceptibility is

$$\chi(0,T) = \left.\frac{dm}{dH}\right|_{H=0} = \frac{d}{dH}\left.\frac{\sinh(H/T)}{\sqrt{\sinh^2(H/T) + e^{-4J/T}}}\right|_{H=0}$$

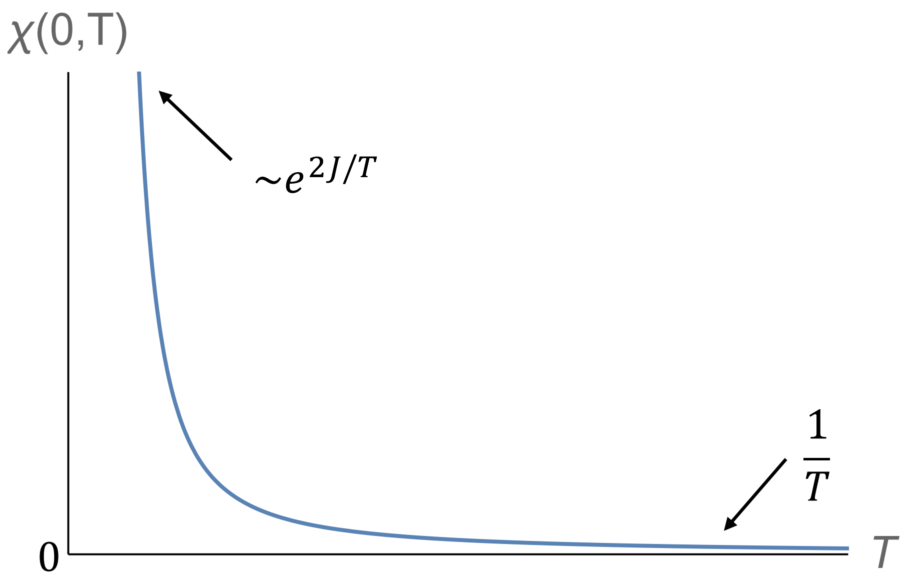
$$\Rightarrow \chi(0,T) = \frac{1}{Te^{-2J/T}} = \frac{e^{2J/T}}{T}$$

And the limits of high- and low-temperature are:

$$\chi(0,T) \sim \begin{cases} \frac{1}{T}, & \text{for } T \gg J \\ \infty, & \text{for } T \to 0 \end{cases}$$

1D Ising Model

$$\chi(0,T) = \frac{e^{2J/T}}{T}$$



At the point $T = 0$ the susceptibility diverges ➡ it is a critical point!
However, there is no magnetic phase, because we cannot have $T < 0$.
This is an example of a so-called “zero-temperature phase transition”.