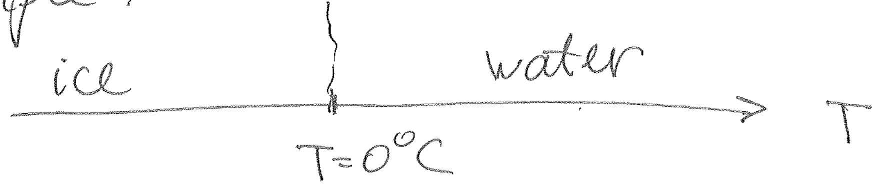
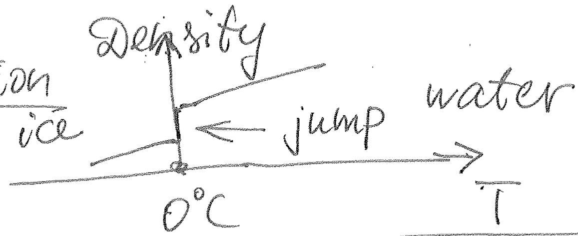
Lecture 8
Phase transitions.
1D - Ising model

With decreasing temperature, a matter can undergo a transition from one to another state.

Example: water $\Leftrightarrow$ ice



First-order phase transition



$\boxed{\text{Symmetry is spontaneously broken at the critical point.}}$

in water : — short-ranged correlations between molecules positions

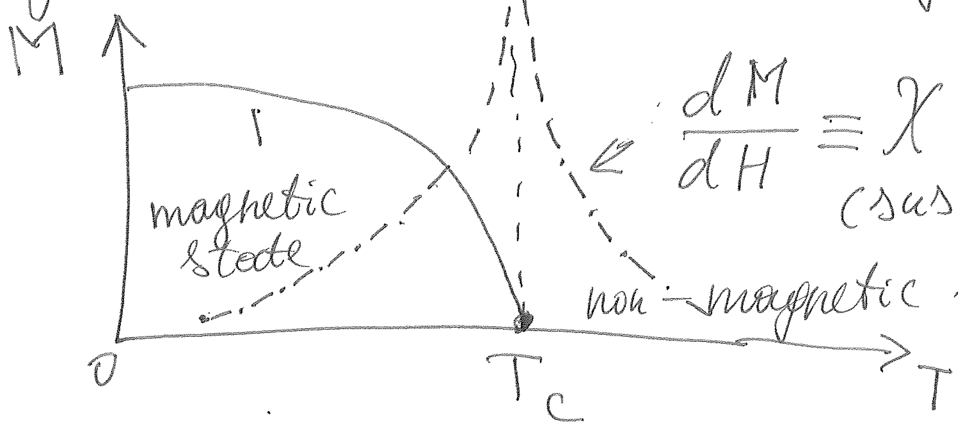
in ice — long-ranged correlations (molecules are arranged regularly)

Magnetic materials.

Transition from non-magnetic to magneti state.

Continuos transitions [2]

Magnetization M versus temperature



Magnetization appears continuosly at $T<T_c$.

$$M \propto (T_c - T)^{\beta}$$

$$\beta = \begin{cases} \frac{1}{8} = 0.125 , & 2D \text{ Ising model} \\ \frac{1}{2} , & D \geq 4 \end{cases}$$

Magnetic susceptibility

$$\chi \equiv \left.\frac{dM}{dH}\right|_{H=0} \propto \frac{1}{|T_c - T|^{\gamma}}$$

$$\gamma = \begin{cases} 7/4 , & 2D\text{-Ising model} \\ 1 , & D>4 , \text{ Ising model} \end{cases}$$

Examples of continuos phase transition

Standard model

gauge symmetric state | broken gauge symmetry Higgs bosons → inflation

Big Bang

t

superconducting state | normal state $R \neq 0$ → T

$R = 0$ T_c

assynchronous state of neurons | ~~[illegible]~~ Brain waves

uncoscious state | cognition →

normal state | epileptic seizure

Prof. Lenz (1920) proposed to his PhD student Ising to solve a model which now we know as the Ising model.

1D - Ising model

We consider a one dimension ~~system~~ lattice or chain of spins with index $n=1, \dots N$

Each spin σ_n takes two values

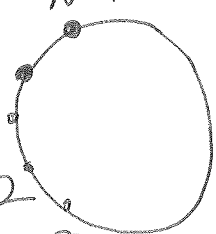
$$\sigma_n = \begin{cases} +1\,, & \text{spin up} \\ -1\,, & \text{spin down} \end{cases}$$

Neighboring spins interact with each other

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

Total energy on a ring

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



$$\sigma_{N+1} \equiv \sigma_1$$

Magnetic field

Energy of a spin in a magnetic field H

$$\text{energy} = -H\sigma_n = \begin{cases} -H, & \sigma_n \parallel H \quad (\sigma_n = +1) \\ +H, & \sigma_n = -1 \quad (\sigma_n \downarrow) \end{cases}$$

1D Ising model in a magnetic field

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

A state of the model is determined by spins

$$(\sigma_1, \sigma_2, \sigma_3, \ldots \sigma_N)$$

Energy

$$E = E(\sigma_1, \sigma_2, \sigma_3 \ldots \sigma_N)$$

Probability to find the system in a state $(\sigma_1 \ldots \sigma_N)$ is

$$w = \frac{1}{Z}\exp\left[-\frac{E(\sigma_1, \sigma_2, \ldots \sigma_N)}{K_B T}\right]$$

The Boltzman constant $K_B = 1$.

Normalization

$$\sum_{\{\text{all possible states}\}}{}' w = 1 \Rightarrow \sum_{\{\sigma_1 = \pm 1,\ \sigma_2 = \pm 1, \ldots\}}{}' w = 1$$

$$\frac{1}{Z}\sum_{\{\sigma_n=\pm1\}}' e^{-E/T} = 1$$

$\Rightarrow$ Partition function

$$Z \equiv \sum_{\{\sigma_n=\pm1\}}' e^{-\frac{E(\sigma_1,\sigma_2\ldots\sigma_N)}{T}}$$

Free energy

$$F = -T\ln Z$$
$$= \underbrace{E}_{\text{internal energy}} - T\underbrace{S'}_{\text{entropy}}$$

Total Magnetization

$$M \doteq \sum_{n=1}^{N}{}' \sigma_n$$

Mean magnetic moment per spins

$$m = \frac{1}{N}\sum_{\{\sigma_n=\pm1\}}' M(\sigma_1\ldots\sigma_N)\,\frac{\exp\left(-\frac{E(\sigma_1\ldots\sigma_N)}{T}\right)}{Z}$$

Note that

$$\sum_{\{\sigma_n=\pm1\}}' = \sum_{\sigma_1=\pm1}'\sum_{\sigma_2=\pm1}'\cdots\sum_{\sigma_N=\pm1}'$$

Note that

$$\langle M\rangle = -\frac{\partial F}{\partial H}$$

Indeed

$$-\frac{\partial F}{\partial H} = \frac{\partial}{\partial H} T\ln Z = \frac{T}{Z}\frac{\partial Z}{\partial H} =$$

$$= \frac{T}{Z}\frac{\partial}{\partial H}\sum_{\{\sigma=\pm1\}} \exp\left[\beta J \sum \sigma_n\sigma_{n+1} + \beta H M\right]$$

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

where $\beta = 1/T$.

Now we will calculate the partition function by use a so-called "the method of transfer matrices".

$$Z = \sum_{\{\sigma_n=\pm1\}} \exp\left[K\sum_{n=1}^{N}\sigma_n\sigma_{n+1} + h\sum_{n=1}^{N}\sigma_n\right]$$

where

$$K \equiv \frac{J}{T}, \quad h \equiv \frac{H}{T}$$

We write

$$\sum_{n=1}^{N}\sigma_n = \sum_{n=1}^{N}\frac{(\sigma_n+\sigma_{n+1})}{2}$$

$$Z = \sum_{\{\sigma_n=\pm 1\}} \exp\left[K \sum_{n}^{N} \sigma_n \sigma_{n+1} + \frac{h}{2} \sum_{n=1}^{N} (\sigma_n + \sigma_{n+1})\right]$$

$$= \sum_{\{\sigma_n=\pm 1\}} \left(\prod_{n=1}^{N} \exp\left[K \sigma_n \sigma_{n+1} + \frac{h}{2}(\sigma_n + \sigma_{n+1})\right] \right)$$

We introduce a matrix $\hat{V}$ with entries

$$V(\sigma_n, \sigma_{n+1}) \equiv \exp\left(K\sigma_n\sigma_{n+1} + \frac{h}{2}(\sigma_n + \sigma_{n+1})\right)$$

This matrix is symmetric

$$V(\sigma_n, \sigma_{n+1}) = V(\sigma_{n+1}, \sigma_n)$$

$$\hat{V} = \begin{pmatrix} V(1,1) & V(1,-1) \\ V(-1,1) & V(-1,-1) \end{pmatrix} =$$

$$= \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}$$

Using this matrix we can write

$$Z = \sum_{\{\sigma_n=\pm 1\}} V(\sigma_1,\sigma_2) V(\sigma_2,\sigma_3) V(\sigma_3,\sigma_4) \ldots V(\sigma_N,\sigma_1)$$

$$= \operatorname{trace}\left(\hat{V}^N\right)$$

Any symmetric matrix can be represented in the form

$$V = P\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} P^{-1}$$

where P is an orthogonal matrix and λ_1 and λ_2 are eigenvalues of $\hat{V}$.
That is λ are solution of equation

$$\lambda \vec{\Psi} = \hat{V}\vec{\Psi} \quad \text{or} \quad (\lambda\hat{I} - V)\vec{\Psi} = 0$$

where $\vec{\Psi} = (\Psi_1, \Psi_2)$ is the eigenvector.
λ are solutions of an equation

$$\det(\hat{V} - \lambda\hat{I}) = 0$$

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

We obtain

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

This gives

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

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

$$\lambda^2 - 2\lambda e^K \cosh h + 2 \sinh 2K = 0$$

$$\left(\lambda - e^{K}\cosh h\right)^2 - e^{2K}\cosh^2 h + e^{2K} - e^{-2K} = 0$$

we use $\cosh^2 x - 1 = \sinh^2 x$

$$\lambda = e^{K}\cosh h \pm \sqrt{e^{2K}\sinh^2 h + e^{-2K}}$$

Two eigenvalues

$$\lambda_1 = e^{K}\cosh h + \sqrt{e^{2K}\sinh^2 h + e^{-2K}}$$

$$\lambda_2 = e^{K}\cosh h - \sqrt{e^{2K}\sinh^2 h + e^{-2K}}$$

Note that

$$\lambda_1 > \lambda_2$$

We use the property $V = \hat{P}\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}\hat{P}^{-1} = \hat{P}\hat{D}\hat{P}^{-1}$

$$\operatorname{tr}\hat{V}^N = \operatorname{tr}\left(\hat{P}\hat{D}\hat{P}^{-1}\cdot\hat{P}\hat{D}\hat{P}^{-1}\cdots P\hat{D}P^{-1}\right)$$

$$= \operatorname{tr}\hat{D}^N = \operatorname{tr}\begin{pmatrix}\lambda_1^N & 0\\ 0 & \lambda_2^N\end{pmatrix} = \lambda_1^N + \lambda_2^N$$

Free energy

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

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

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

Taking into accout that $\lambda_1 > \lambda_2$ we have

$$\lim_{N\to\infty} \left(\frac{\lambda_2}{\lambda_1}\right)^N \to 0$$

Therefore, at $N \gg 1$

$$\mathcal{F} = -TN \ln \lambda_1$$

Free energy per spin $f = f(T,H)$

$$f = \frac{1}{N}\mathcal{F} = -T \ln \lambda_1$$

We obtain

$$f = -T \ln \left[e^{K} \cosh h + \left(e^{2K} \sinh^2 h + e^{-2K} \right)^{1/2} \right]$$

Recall that $K = \beta J$, $h = \beta H$.

Magnetic moment

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

Thus

$$m = \frac{\partial}{\partial h} \ln \left[e^{K} \cosh h + \left(e^{2K} \sinh^2 h + e^{-2K} \right)^{1/2} \right]$$

$$= \frac{e^{K} \sinh h + \frac{1}{2}\left(2 e^{2K} \sinh h \cosh h\right)/\sqrt{}}{[\ldots]}$$

$$= \frac{e^{K}\sinh h \,\cancel{\left[\sqrt{\dots} + e^{K}\cosh h\right]}}{\left[e^{2K}\sinh^2 h + e^{-2K}\right]^{1/2}\cancel{\left[e^{K}\cosh h + \sqrt{\dots}\right]}}$$

Thus the magnetic moment is

$$m(T,H) = \frac{e^{K}\sinh h}{\left[e^{2K}\sinh^2 h + e^{-2K}\right]^{1/2}}$$

$$\boxed{m(T,H) = \frac{\sinh h}{\left[\sinh^2 h + e^{-4K}\right]^{1/2}}}$$

Small magnetic field

$$h = \frac{H}{T} << 1$$

$$m(T,H) \cong \frac{h}{(h^2 + e^{-4K})^{1/2}} = \frac{H}{(H^2 + T^2 e^{-4K})^{1/2}}$$

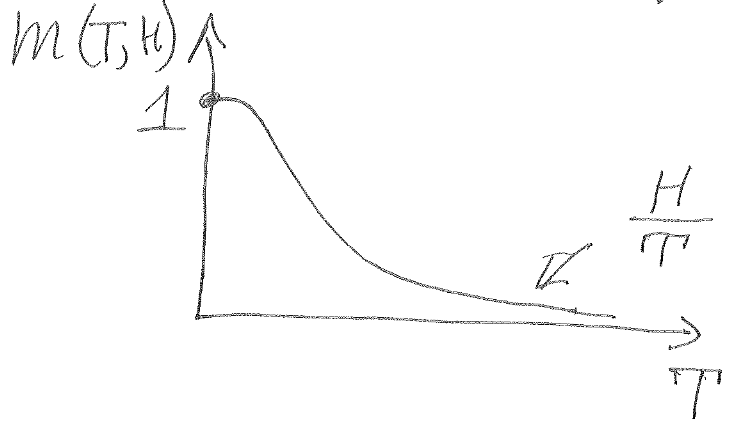
i.e., $m \propto H$

The case $T \to 0$, $h = H/T >> 1$

then $e^{-4K} \ll \sinh^2 h$

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

13



Large temperature $T \gg J$, i.e. $K = \frac{J}{T} \ll 1$, then

$$m(T,H) \simeq \frac{H}{(H^2+T^2)^{1/2}} \approx \frac{H}{T}$$

Susceptibility

$$\chi(T,H) = \frac{dm}{dH}$$

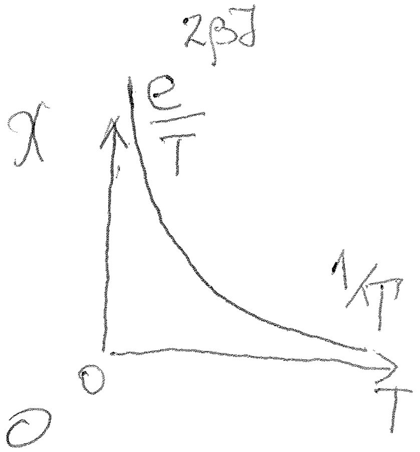
Zero-field susceptibility

$$\chi(T,0) = \left.\frac{dm}{dH}\right|_{h=0} = \frac{d}{dH}\left(\frac{H}{(H^2+T^2e^{-4K})^{1/2}}\right)$$

$$= \frac{1}{Te^{-2K}}$$

We get

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



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