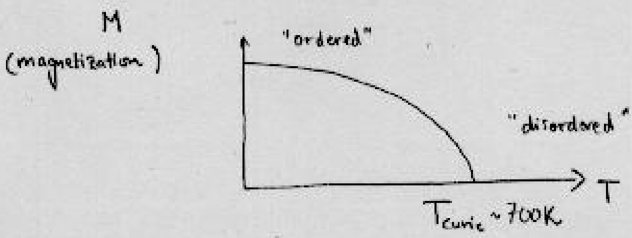
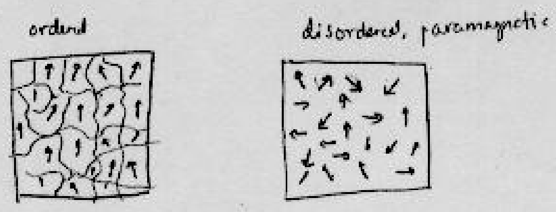
Spin models

($\Rightarrow$ a review of many basic concepts of statistical physics.)

Physics background

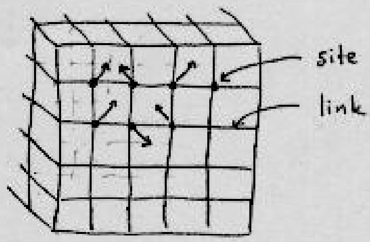
How does a ferromagnet behave as a function of the temperature T?





Definition

Model the system by a three-dimensional lattice;
Assign spins to lattice "sites".



$\nearrow$ = spin vector $\bar{S}_i$, living at site i.

The energy of the system: model by nearest-neighbour couplings only.

$$E = \text{const.} - J \sum_{\langle ij \rangle} \bar{S}_i \cdot \bar{S}_j$$

; $J > 0$ for ferromagnets; $\langle ij \rangle$ = nearest neighbours, counted once only.

If there is an external magnetic field $\bar{H}$ present:

$$\delta E = - \gamma \bar{H} \cdot \sum_i \bar{S}_i$$

; $\gamma \bar{S}_i$ = magnetic moment

$\Rightarrow$ spins like to align with each other and with $\bar{H}$.

Thermodynamics

The properties of the system at finite temperatures are encoded in its partition function Z:

$$Z = \mathrm{Tr}\, e^{-\frac{\hat{H}}{k_B T}} \quad , \quad \hat{H} = \text{Hamiltonian}$$

$$= \sum_n e^{-\frac{E_n}{k_B T}} \quad , \quad E_n = \text{energy eigenvalues} .$$

Let us simplify the notation by

- leaving out the inessential "const." from E.
- defining new dimensionless couplings. There are many different conventions in the literature. We choose

$$\beta \equiv \frac{J}{k_B T} \quad , \quad \bar{h} \equiv \frac{g \bar{H}}{k_B T}$$

- denote by N_{tot} the total number of spins.

$$\Rightarrow \quad \boxed{Z(\beta, \bar{h}, N_{tot}) = \sum_{\{\bar{s}_i\}} \exp\left[\beta \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j + \bar{h} \cdot \sum_i \bar{s}_i \right]}$$

"Thermodynamic limit" corresponds to an infinite number of degrees of freedom: $N_{tot} \to \infty$.

"Free energy": $\quad Z \equiv e^{-\beta F}$

$$\Leftrightarrow \quad F = -\frac{1}{\beta} \ln Z \qquad \text{(again in specific units)}$$

Generalizations

A large variety of different spin models can be defined by:

- changing the dimensionality d of the lattice. Each site has $2d$ nearest-neighbours. In ferromagnets, $d = 3$.

$$\sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j = \sum_{\bar{x}} \sum_{i=1}^{d} \bar{s}_{\bar{x}} \cdot \bar{s}_{\bar{x}+\hat{\imath}} \quad , \quad \bar{x} = (x_1, \dots, x_d) \; , \; \hat{\imath} = \text{unit vector in direction } i .$$

- changing the nature of the spin variables $\bar{s}_i$:

(i) Ising model: $\bar{s}_i \to z_i \equiv \pm 1$.

The scalar variables z_i could be thought of e.g. as the z-components of the spin of spin-$\frac{1}{2}$ particles.

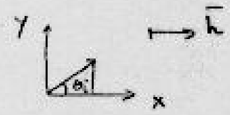
$$Z = \prod_{k=1}^{N_{tot}} \sum_{z_k=-1}^{+1} \exp\left[\beta \sum_{\langle ij \rangle} z_i z_j + h \sum_i z_i \right] .$$

The same system can be written in other forms: say, $z_i \to \hat{z}_i = \frac{z_i + 1}{2}$ so that the spins are $0, 1$.

(ii) q-state Potts model: $\bar{s}_i \to z_i = 1, 2, \dots, q$,

$$Z = \prod_{k=1}^{N_{tot}} \sum_{z_k=1}^{q} \exp\left[\beta \sum_{\langle ij \rangle} \delta(z_i, z_j) \right] \quad , \quad \delta = \text{Kronecker delta-function}$$

(iii) XY-model, or $O(2)$-symmetric model:



$$\bar{s}_i \equiv s_{ix} \hat{e}_x + s_{iy} \cdot \hat{e}_y \, , \quad |\bar{s}_i| = 1$$

$$\bar{s}_i \cdot \bar{s}_j = \cos(\theta_i - \theta_j)$$

$$Z = \prod_{k=1}^{N_{tot}} \int_{-\pi}^{\pi} \frac{d\theta_k}{2\pi} \exp\left[\beta \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) + |\bar{h}| \sum_i \cos\theta_i \right]$$

(iv) Heisenberg-model, or $O(3)$-symmetric model:

What we had for ferromagnets, i.e. three-dimensional (unit) vectors $\bar{s}_i$.

(v) $O(N)$-model: $\quad \bar{s}_i \in S^{N-1} = \left\{ \bar{x} \in \mathbb{R}^N, \; |\bar{x}| = 1 \right\}$

So $\bar{s}_i$ is an N-component unit vector.

Note that N and d are completely independent!

$$Z = \prod_{k=1}^{N_{tot}} \int_{S^{N-1}} d\bar{s}_k \; \exp\left[\beta \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j + \bar{h} \cdot \sum_i \bar{s}_i \right]$$

Observables

Rather than Z directly, observations concern some of Z's derivatives.

- expectation value of energy:

$$\langle E \rangle = \left\langle -\sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j \right\rangle = -\frac{\partial}{\partial \beta} \ln Z = \frac{\partial}{\partial \beta} (\beta F).$$

- magnetization:

$$\langle M \rangle = \left\langle \frac{\bar{h}}{|\bar{h}|} \cdot \sum_i \bar{s}_i \right\rangle = \frac{\partial}{\partial |\bar{h}|} \ln Z$$

- specific heat / heat capacity:

$$\chi_E = -\frac{\partial}{\partial \beta} \frac{\langle E \rangle}{N_{tot}} = \frac{1}{N_{tot}} \frac{\partial^2}{\partial \beta^2} \ln Z$$

$$= \frac{1}{N_{tot}} \frac{\partial}{\partial \beta} \cdot \frac{\int \{\bar{s}_i\} \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j \exp[\cdots]}{Z}$$

$$= \frac{1}{N_{tot}} \left\{ \frac{\int \{\bar{s}_i\} \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j \sum_{\langle kl \rangle} \bar{s}_k \cdot \bar{s}_l \exp[\ ]}{Z} - \left(\frac{\int \{\bar{s}_i\} \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j \exp[\cdots]}{Z} \right)^2 \right\}$$

$$= \frac{1}{N_{tot}} \left\{ \langle E^2 \rangle - \langle E \rangle^2 \right\} = \frac{1}{N_{tot}} \langle (\Delta E)^2 \rangle \quad ; \Delta E = E - \langle E \rangle$$

- magnetic susceptibility / permeability:

$$\chi_M = \frac{\partial}{\partial |\bar{h}|} \frac{\langle M \rangle}{N_{tot}} = \frac{1}{N_{tot}} \frac{\partial^2}{\partial |\bar{h}|^2} \ln Z$$

$$= \frac{1}{N_{tot}} \langle (\Delta M)^2 \rangle \quad ; \quad \Delta M = M - \langle M \rangle$$

Specific heat [illegible] denoted by χ_E, magnetic susceptibility / permeability by χ_M.

- correlation lengths ξ:

$$\lim \left[\langle O_{\bar{x}} O_{\bar{y}} \rangle - \langle O_{\bar{x}} \rangle \langle O_{\bar{y}} \rangle \right] = \text{Polynomial}(|\bar{x}-\bar{y}|) \cdot \exp\left(-\frac{|\bar{x}-\bar{y}|}{\xi} \right)$$

An example of a solution : $d=1$ Ising model

(Exact solution known also for $d=2$: Onsager '44 for $\bar{h}=0$, C.N. Yang '52 for $\bar{h}\neq 0$).

Impose periodic boundary conditions : $z_{N_{tot}}$, z_1 z_2 z_3 $\cdots$

$$\beta \sum_{\langle ij \rangle} z_i z_j + h \sum_i z_i = \beta \sum_{i=1}^{N_{tot}} z_i z_{i+1} + \frac{1}{2} h \sum_{i=1}^{N_{tot}} (z_i + z_{i+1}) \quad ; \quad z_{N_{tot}+1} \equiv z_1$$

Consider a 2×2 matrix $T_{zz'}$, with

$$T_{zz'} = \exp\left[\beta z z' + \tfrac{1}{2} h (z+z') \right]$$

Then

$$Z = \sum_{z_1=\{-1,+1\}}^{+1} \sum_{z_2=\{-1,+1\}}^{+1} \cdots \sum_{z_{N_{tot}}=\{-1,+1\}}^{+1} T_{z_1 z_2} T_{z_2 z_3} \cdots T_{z_{N_{tot}} z_1}$$

$$= \sum_{z_1=\{-1,+1\}} \left(T^{N_{tot}}\right)_{z_1 z_1} = \mathrm{Tr}\left[T^{N_{tot}}\right],$$

where
$$T = \begin{pmatrix} e^{\beta+h} & e^{-\beta} \\ e^{-\beta} & e^{\beta-h} \end{pmatrix}$$

The matrix can be diagonalised: $T = S^{-1} \begin{pmatrix} \lambda_+ & \\ & \lambda_- \end{pmatrix} S$, where the eigenvalues are

$$\lambda_\pm = e^{\beta} \left[\cosh(h) \pm \sqrt{\sinh^2(h) + e^{-4\beta}} \right]$$

$$\ln Z = \ln \mathrm{Tr}\left[T^{N_{tot}}\right] = \ln \mathrm{Tr} \begin{pmatrix} \lambda_+^{N_{tot}} & \\ & \lambda_-^{N_{tot}} \end{pmatrix} = \ln \left[\lambda_+^{N_{tot}} \left(1 + \left(\frac{\lambda_-}{\lambda_+}\right)^{N_{tot}} \right) \right]$$

$$= N_{tot} \ln \lambda_+ + \ln \left(1 + \left(\frac{\lambda_-}{\lambda_+}\right)^{N_{tot}} \right)$$

Since $0 < \frac{\lambda_-}{\lambda_+} < 1$, $\lim_{N_{tot}\to\infty} \left(\frac{\lambda_-}{\lambda_+}\right)^{N_{tot}} = 0$, and the latter term does not contribute.

Average magnetization:

$$\frac{\langle M \rangle}{N_{tot}} = \frac{\partial}{\partial h} \frac{1}{N_{tot}} \ln Z = \frac{\partial}{\partial h} \ln \lambda_+$$

$$= \frac{\sinh(h) + \dfrac{\sinh(h)\cosh(h)}{\sqrt{\sinh^2(h) + e^{-4\beta}}}}{\cosh(h) + \sqrt{\sinh^2(h) + e^{-4\beta}}}$$

$$= \frac{\sinh(h)}{\sqrt{\sinh^2(h) + e^{-4\beta}}}$$