

Classical spin models

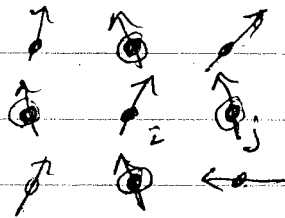
$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \quad \text{simple model of interacting magnetic}$$

classical spins $\vec{S}_i$ of unit magnitude $|\vec{S}_i| = 1$ on sites i of a periodic d -dimensional lattice.

$\vec{S}_i$ interacts only with its neighbors $\vec{S}_j$.

$\langle i,j \rangle$ indicates nearest neighbor bonds of the lattice.

If coupling $J > 0$, then ferromagnetic interaction i.e. spins are in lower energy state when they are aligned.



$\vec{S}_i$ interacts with spins on sites labeled by $\odot$.

Behavior of model depends significantly on dimensionality of lattice d , and number of components of the spin $\vec{S}$ n .

Examples: $\vec{S} = (S_x, S_y, S_z)$ points in 3-dimensional space
 $\underline{n=3}$ called the Heisenberg model

$\vec{S} = (S_x, S_y)$ restricted to lie in a plane
 $\underline{n=2}$ called the XY model

$S = S_z = \pm 1$ restricted to lie in one direction
 $\underline{n=1}$ called the Ising model

less obvious $\left\{ \begin{array}{l} \underline{n=0} \\ \underline{n=\infty} \end{array} \right.$ called the polymer model
called the spherical model

We will focus on the Ising model (1925)

$$S = \pm 1$$

Ensembles

① fixed magnetization $M = \sum_i S_i$ M is total magnetization

partition function $\tilde{Z}(T, M) = \sum_{\{S_i\}} e^{-\beta \mathcal{H}[S_i]}$
s.t. $\sum_i S_i = M$

sum over all spin configurations

obeying the constraint $\sum_i S_i = M = N^+ - N^-$

$\uparrow$ # up spins $\uparrow$ # down spins

(similar to canonical ensemble with $\sum_i n_i = N$ total # particles)

Helmholtz free energy $F(T, M) = -k_B T \ln \tilde{Z}(T, M)$

② fixed magnetic field

to remove constraint of fixed M we can Legendre transform to a conjugate variable h , the magnetic field.

Gibbs free energy $G(T, h) = F(T, M) - h M$

$$\Rightarrow \left(\frac{\partial F}{\partial M} \right)_T = h \quad \text{and} \quad \left(\frac{\partial G}{\partial h} \right)_T = -M$$

$$dF = -SdT + h dM \quad \text{and} \quad dG = -SdT - Mdh$$

$\uparrow$ entropy $\uparrow$ entropy

To get partition function for G , take Laplace transform of $\tilde{Z}$

$$Z(T, h) = \sum_M e^{\beta h M} \tilde{Z}(T, M)$$

$$= \sum_M e^{\beta h M} \sum_{\{s_i\}} e^{-\beta H[s_i]} \text{ s.t. } \sum_i s_i = M$$

$$Z(T, h) = \sum_{\{s_i\}} e^{-\beta [H[s_i] - h \sum_i s_i]}$$

← looks like interaction of magnetic field h with total magnetization $M = \sum_i s_i$

τ unconstrained sum over all spin configs $\{s_i\}$
(similar to grand canonical ensemble with $\sum_i n_i = N$ unconstrained)

$$G(T, h) = -k_B T \ln Z(T, h)$$

Check:

$$\frac{\partial G}{\partial h} = -k_B T \frac{\partial Z}{Z \partial h} = -k_B T \sum_{\{s_i\}} \frac{\partial}{\partial h} \left(e^{-\beta [H - h \sum_i s_i]} \right)$$

$$= -k_B T \sum_{\{s_i\}} e^{-\beta [H - h \sum_i s_i]} (\beta \sum_i s_i)$$

$$= - \frac{\sum_{\{s_i\}} e^{-\beta [H - h \sum_i s_i]} (\sum_i s_i)}{\sum_{\{s_i\}} e^{-\beta [H - h \sum_i s_i]}}$$

$$= -\langle \sum_i s_i \rangle = -M \quad \text{so } \frac{\partial G}{\partial h} = -M \text{ as required}$$

we can work in fixed magnetization or fixed magnetic field ensemble according to our convenience. Usually it is easiest to work with fixed magnetic field. In this case we usually write

$$H = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$$

including the magnetic field part in the definition of H .

$$Z = \sum_{\{S_i\}} e^{-\beta H} \quad \nwarrow \text{includes } h \text{ term}$$

define magnetization density

$$m = \frac{M}{N} = \frac{1}{N} \left\langle \sum_i S_i \right\rangle \quad N = \text{total number spins}$$

Helmholtz free energy density: In limit $N \rightarrow \infty$, $F(T, M) = N f(T, m)$

$$\frac{F}{N} \equiv f(T, m) \quad \text{depends on magnetization density}$$

$$df = -s dT + h dm \quad s = \frac{S}{N} \quad \text{entropy per spin}$$

Gibbs free energy density: In limit $N \rightarrow \infty$, $G(T, h) = N g(T, h)$

$$\frac{G}{N} \equiv g(T, h)$$

$$dg = -s dT - m dh$$

$$\left(\frac{\partial f}{\partial m} \right)_T = h \quad , \quad \left(\frac{\partial g}{\partial h} \right)_T = -m$$

What behavior do we expect from Ising model?

For a given h , what is the resulting $m(T, h)$?

For $h > 0$, expect $m > 0$ as energetically favorable for spins to align parallel to h .

For $h < 0$, similarly expect $m < 0$.

In general, $m(T, -h) = -m(T, h)$, since Hamiltonian has the symmetry $H[s_i, h] = H[-s_i, -h]$

What if $h = 0$?

As $T \rightarrow \infty$ we expect each spin to be random so $m \rightarrow 0$.

But even at finite T we might expect $m = 0$ because of symmetry: $H[s_i, 0] = H[-s_i, 0]$ so a configuration $\{s_i\}$ in the partition function sum will enter with the same weight as the configuration $\{-s_i\}$ and so expect $\langle s_i \rangle = 0$.

But at $T = 0$, the system has two degenerate ground states: all up or all down, with $m = \pm 1$. The ground state breaks the symmetry of the Hamiltonian.

More specifically: $\lim_{h \rightarrow 0^+} \lim_{T \rightarrow 0} m(T, h) = +1$

limit $h \rightarrow 0$ from above

limit $h \rightarrow 0$ from below $\rightarrow \lim_{h \rightarrow 0^-} \lim_{T \rightarrow 0} m(T, h) = -1$

Can one have such a broken symmetry state at finite T ?

$$\text{ie } \lim_{h \rightarrow 0^+} m(T, h) = m > 0$$

$$\lim_{h \rightarrow 0^-} m(T, h) = m < 0$$

For a finite size system, N finite, the answer is NO!

For a finite size system, the energy $H[s_i]$ is always finite. The statistical weight of $\{s_i\}$ will always be equal to that of $\{-s_i\}$ in a small h , as we take $h \rightarrow 0$

However, in the thermodynamic limit $N \rightarrow \infty$, the answer can be Yes! Now the energy of states with a finite $\sum_i s_i$ will grow infinitely large as N . The statistical weight of config $\{s_i\}$ can be infinitely different from that of $\{-s_i\}$ in a small h , even if take $h \rightarrow 0$. ($\infty \times 0 \neq 0$)

$H[s_i] - H[-s_i] \propto hN$ does not necessarily vanish as $h \rightarrow 0$, if $N \rightarrow \infty$ first.

It is possible that at finite T

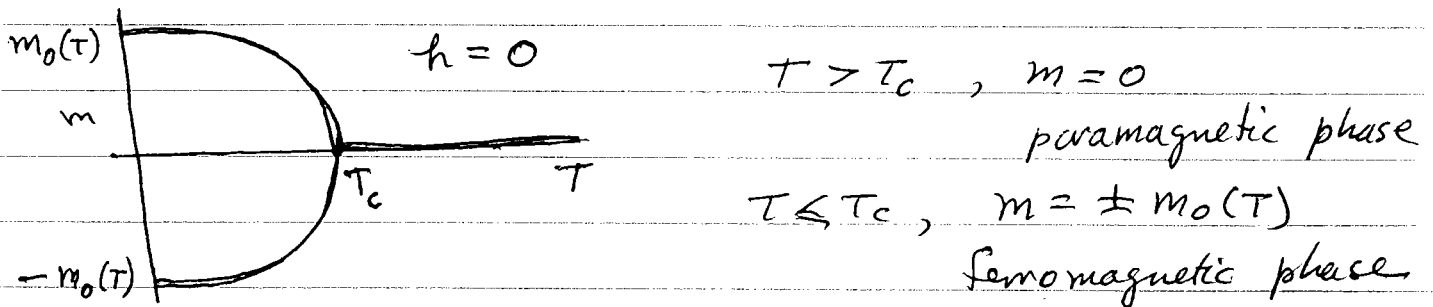
$$\lim_{h \rightarrow 0^+} \left[\lim_{N \rightarrow \infty} m(T, h) \right] = m > 0$$

$$\lim_{h \rightarrow 0^-} \left[\lim_{N \rightarrow \infty} m(T, h) \right] = m < 0$$

It is important to take the limits in the above order - ie first take $N \rightarrow \infty$ in a finite h , and then take $h \rightarrow 0$. Reversing the limits ($h \rightarrow 0$ first, then $N \rightarrow \infty$) gives $m=0$ by symmetry of H .

If such broken symmetry states exist at finite T , then do they persist at all T ? or do they disappear at a well defined T_c ?

Possibility of a phase transition

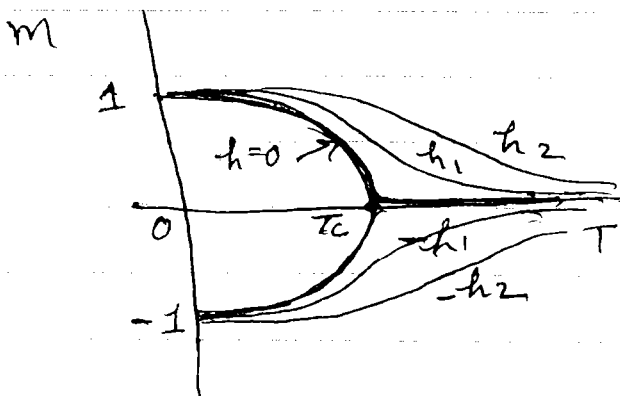


$m(T, 0)$ is singular at $T = T_c$

T_c is ferromagnetic phase transition

The ordered state at $T \leq T_c$ is a state of spontaneously broken symmetry. In $h=0$ the system will pick either the up or the down state to order in, breaking the symmetry of the Hamiltonian.

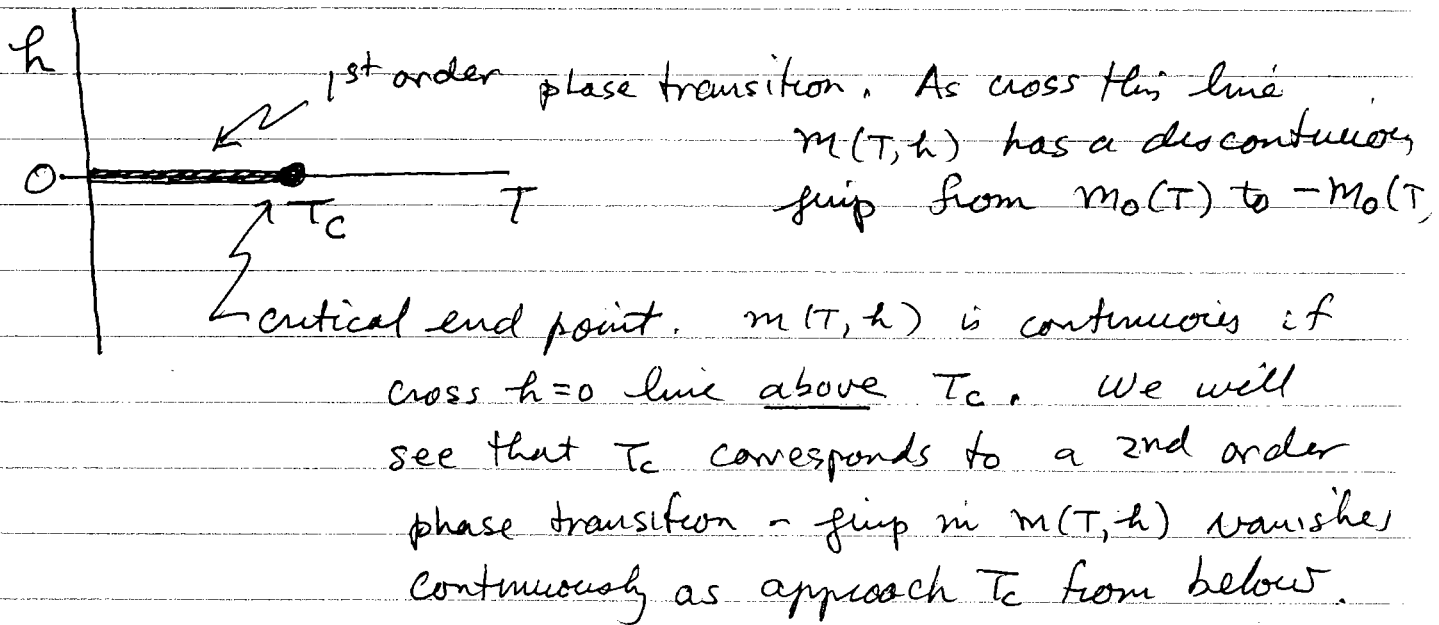
At finite h , expect $m(T, h)$ to behave like



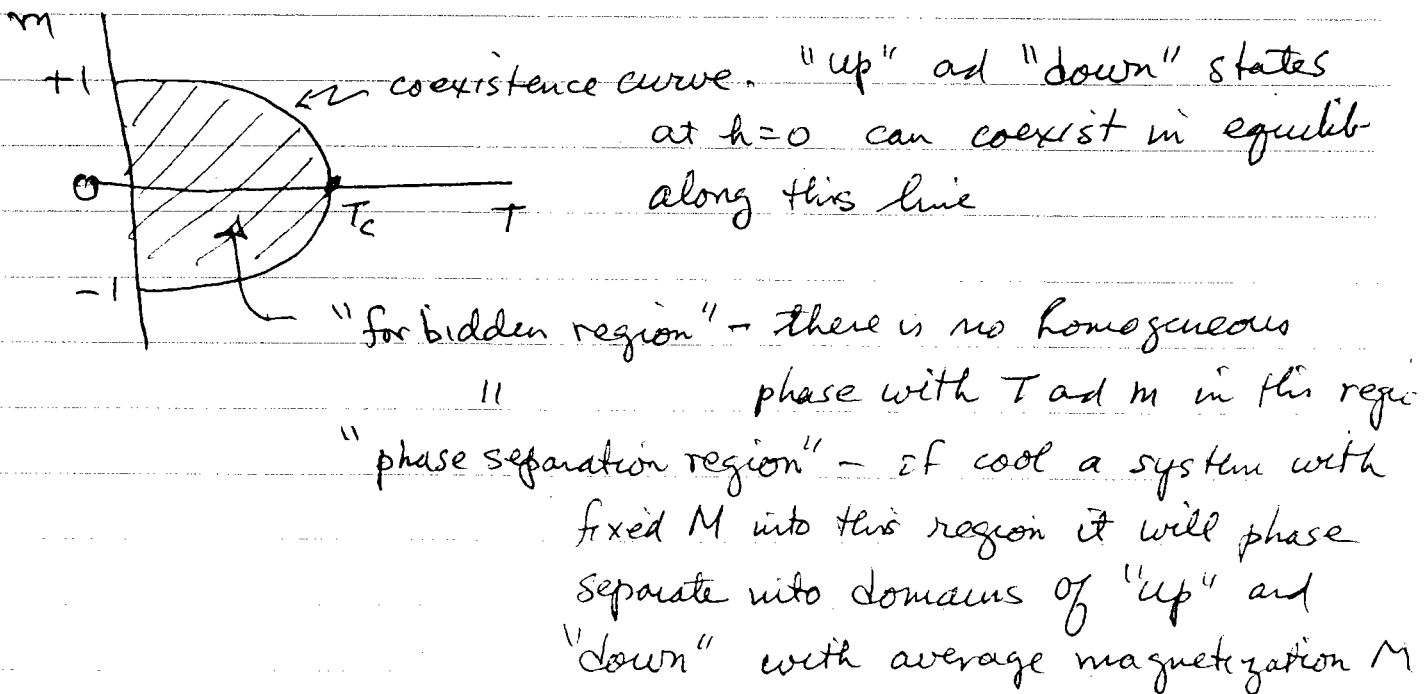
$h_1 < h_2$

$m(T, h)$ is smooth function of T for $h \neq 0$

Phase diagram in h - T plane



Phase diagram in m - T plane



Many similarities to liquid-gas phase diagram

We said that to have a state of spontaneously broken symmetry at finite T ~~requires~~, one needs to be in thermodynamic limit $N \rightarrow \infty$.

Similarly, true singular phase transitions can only occur in this $N \rightarrow \infty$ limit. Proof as follows:
partition function sum:

$$Z(T, h) = \sum_{\{s_i\}} e^{-\beta H[s_i]}$$

For finite system (N finite) the number of configurations to sum over is 2^N is finite

Z is therefore the sum of a finite number of analytic functions ("analytic" here in the sense of complex function theory - has no singularities as vary T, h). As such, Z must itself be an analytic function of T and h .

$\Rightarrow Z$ can have no singularities

$\Rightarrow$ no singularities in any thermodynamic quantities

$\Rightarrow$ no phase transitions.

Only in thermodynamic limit of $N \rightarrow \infty$ is Z now the sum of an infinite ~~small~~ number of analytic functions. Such an infinite sum need NOT be analytic, so phase transitions can exist.