STAT MECH – PHASE TRANSITIONS – Illustrated with Ising model

Ising model – N spins on square lattice

$$E_v = -\sum_{i}^{N} H\mu s_i - J\sum_{i,j}{}' s_i s_j$$

$$s_i = \pm 1$$

J > 0, favorable for spins to align

' $\Rightarrow$ nearest neighbor only

oftentimes written *i < j* or with a factor of ½

Ph.D. thesis of E. Ising (1925) solved 1D

2D solved by Onsager (1944)

J > 0 ferromagnetic

J < 0 antiferromagnetic

Magnetization

$$\langle M \rangle = \sum_{i=1}^{N} \mu s_i$$

$T_c =$ curie temp

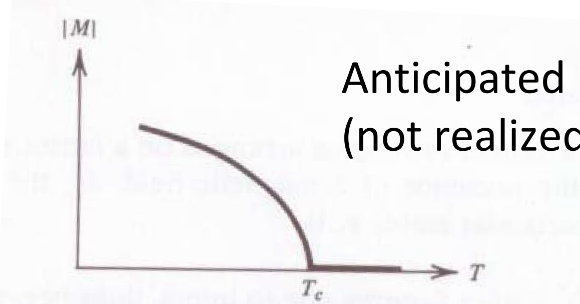


Fig. 5.2. Spontaneous magnetization.

Anticipated behavior (not realized in 1D)

(from Chandler)

suppose *H = 0*

lowest energy = *-DNJ* (*D* = dimension)

$$\left(s_{N+1} = s_1\right)$$

$$\left.\begin{array}{ll} 1D & 2 \\ 2D & 4 \\ 3D & 6 \end{array}\right]$$ # nearest neighbor spins

$$Q = \sum_{v} e^{-\beta E_v} = \sum_{s_{1=\pm1}} \cdots \sum_{s_{N=\pm1}} e^{\left[\beta\mu H \sum_{i=1}^{N} s_i + \beta J \sum_{ij}^{N}{}' s_i s_j\right]}$$

1-D lattice

the interaction energy involves a single sum

$-J \sum_{i=1}^{N} s_i s_{i+1}$, with periodic boundary conditions

$$H = 0 \rightarrow Q = 2N\left\{\left[\cosh\left(\beta J\right)\right]^N + \left[\sinh\left(\beta J\right)^N\right]\right\}$$

$$\approx \left[2\cosh\left(\beta J\right)\right]^N$$

2 spin-linear chain

$$e^{\beta J\left(s_1 s_2 + s_2 s_3\right)}$$

$s_1 s_2$	
1 1	$e^{\beta(2)}$
1-1	$e^{-\beta(2)}$
-1 1	$e^{-\beta(2)}$
-1-1	$e^{\beta(2)}$

No spontaneous magnetization in 1D

$$\uparrow \quad \uparrow \cdots \uparrow \cdots \uparrow$$

1 2 N

$$E = -NJ$$

flip part of the chain

$$\uparrow \quad \uparrow \cdots \downarrow \cdots \downarrow$$

1 2 N

$$E = (-N + 4)J$$

recall PBC

small energy difference between a magnetic and
non-magnetic systems

So, for large *N*, even at very low *T*, there is no
net magnetization

(Actually, even if it were not for this issue, there is
the problem of the degenerate ground state.)

For a 2-D spin system

… ↑ ↑ ↑ ↑ …

↑ ↑ ↑ ↑

… ↓ ↓ ↓ ↓ …

↓ ↓ ↓ ↓

the cost for flipping one half the spins energy goes as $\sqrt{N}$ when starting with fully aligned spin system.

Onsager solved analytically the 2D Ising problem

$$H = 0, \quad Q = \left[2\cosh(2\beta J) e^{I} \right]^{N}$$

$$I = \frac{1}{2\pi}\int_0^{\pi} d\varphi \ell n \left\{ \frac{1}{2}\left[1 + \left(1 - \kappa^2 \sin^2 \varphi \right) \right]^{1/2} \right\}$$

$$\kappa = 2\sinh(2\beta J) / \cosh^2(2\beta J)$$

depending on definition of *J*, need to divide by 2 to prevent double counting

Spontaneous magnetism for $T < T_c = \dfrac{2.269J}{k}$

$\uparrow$

$$\sinh\left(\frac{2J}{kT_c}\right) = 1$$

near T_c

$$C / N \sim \frac{8k}{\pi}\beta J \ell n\left|\frac{1}{T - T_c}\right|$$

$$M / N \sim \text{ constant } \left(T_c - T\right)^{1/8},\ T < T_c$$

Corrected exponent

3D from numerical solution

near T_c

$$C / N \sim \frac{1}{\left(T - T_c\right)^{1/8}}$$

$$M / N \sim \left(T_c - T\right)^{0.313},\ T < T_c$$

critical exponents
depend on dimensionality

Connection between Ising and Lattice-Gas Models

Lattice gas

cell occupied $n_i = 1$

cell empty $n_i = 0$

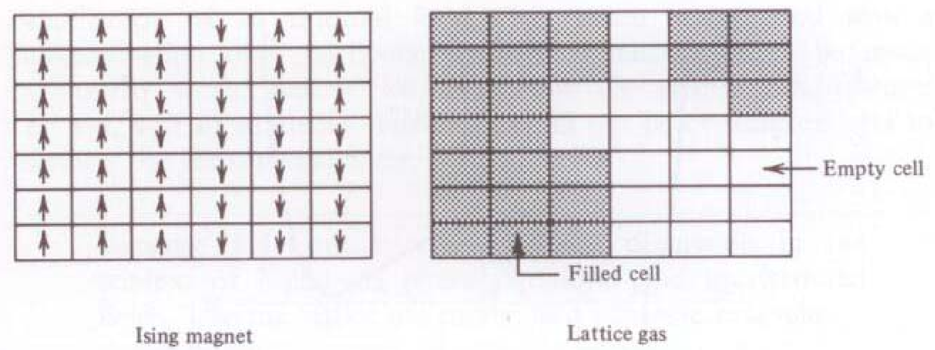


Fig. 5.3 from Chandler

particles in adjacent cells energy = $-\varepsilon$

$$E = -\varepsilon \sum_{i,j}{}' n_i n_j$$

$$\Xi = \sum_{n_1,\ldots n_M}^{N} e^{\left\{\beta\mu\sum n_i + \beta\varepsilon\sum' n_i n_j\right\}}$$

sums over # cells

Lattice gas model is isomorphic with Ising model

$$s_i \rightarrow 2n_i - 1$$

spin up $\rightarrow$ occ site
spin down $\rightarrow$ empty site
mag field $\rightarrow$ chemical potential

$$J \rightarrow \varepsilon / 4$$

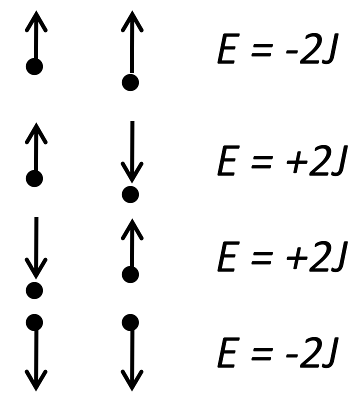
Ising model – broken symmetry

all spins up and all spins down same energy

$$\langle M \rangle = \frac{1}{Q} \sum_{v} \left(\sum_{i=1}^{N} \mu s_i \right) e^{-\beta E v}$$

for every configuration with net up spin
there is another with equal down spin

so why should we ever see magnetization?



$$Q = 2e^{2\beta J} + 2e^{-2\beta J}$$

$$\langle M \rangle = \frac{\mu \left[2e^{2\beta J} + 0e^{2\beta J} - 2e^{-2\beta J} \right]}{Q}$$

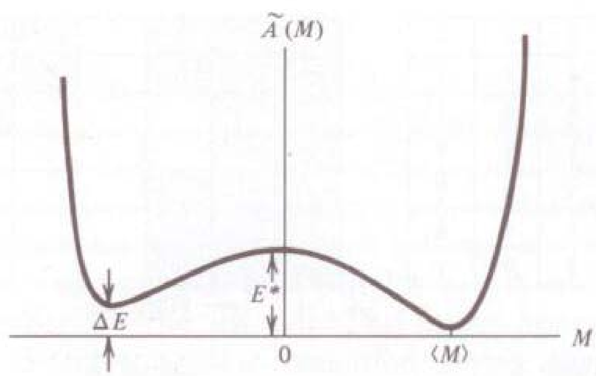


fig. 5.4 from Chandler

$$\tilde{Q}(M) = \sum_{\nu} \Delta(M - M_{\nu}) e^{-\beta E_{\nu}}$$

Fluctuations between <*M*> and -<*M*> vanishingly small for large system

$$\Delta(M - M_{\nu}) = 1, \quad M = M_{\nu}$$
$$= 0, \quad M \neq M_{\nu}$$

add weak field $\rightarrow$ magnetize
remove field $\rightarrow$ spontaneous fluctuations do not destroy broken symmetry
M can be viewed as an order parameter

Question boils down to:

Does the system have long-range order?

Pair correlation function

$$c_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$$

= 0 if spin at *i* uncorrelated with that of *j*.

$$\sum_{j=2}^{N} c_{1j} =$$ # of spins correlated with spin 1.

Susceptibility $\chi = \frac{1}{N}\left(\frac{\partial \langle M \rangle}{\partial(\beta H)}\right)_\beta$

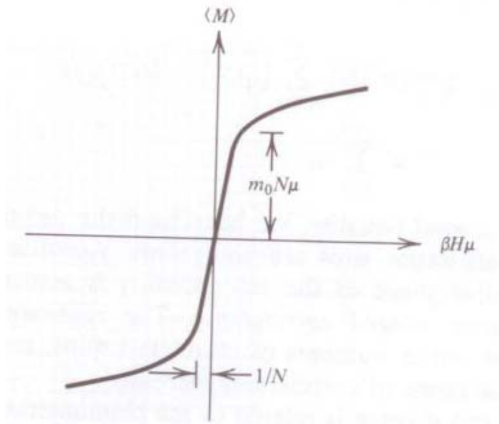
$$\delta M = M - \langle M \rangle$$

$$= \mu \sum_{i=1}^{N} \left[s_i - \langle s_i \rangle \right]$$

$$\chi = \frac{1}{N}\left\langle (\delta M)^2 \right\rangle$$

$$\chi = \frac{\mu^2}{N} \sum_{i,j} \left[\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \right] = \mu^2 \sum_{i=1}^{N} c_{1j}$$

using fact all sites are equivalent



<*M*> for finite *N*
fig. from Chandler

$T < T_c$

<*M*> jumps at *H = 0*, so $\dfrac{\partial \langle M \rangle}{\partial H}$ diverges.

suppose *N* large but not ∞, *H = 0, and* $T < T_c$

$$\langle s_i \rangle = 0$$

$$\sum_{j=1}^{N} \langle s_i s_j \rangle = N m_0$$

$$\chi = N m_0 \mu^2$$

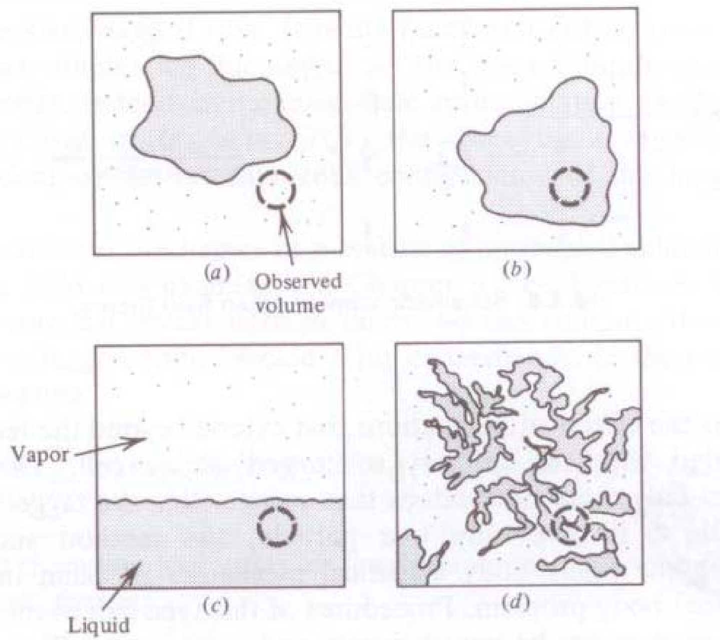
(0 $\Rightarrow$ zero field)

Under the stated conditions
the choice of s1 (+ or -)
biases the other spins

divergence of $\chi \Leftrightarrow$ macroscopic fluctuations

quenched by applying a small symmetry-breaking field

χ also diverges near the critical point
now no difference between spin up/down
(barrier disappears)



Fluctuations for liq.-vapor equilibria (from Chandler). (a), (b), $T << T_c$; (c) $T < T_c$, with gravitational field; (d) $T \approx T_c$