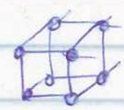
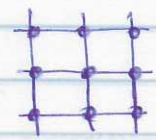
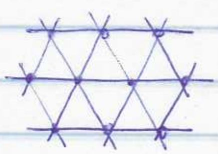
Lattice models and their phase transitions

(Roughly, 6.1–6.2 in Kardar v.2
worked problems in chapter 1)

– want to give more concrete examples and motivation before developing effective field theory description

Models of magnetism: atoms with magnetic moment (e.g. atom with an unpaired electron) forming a periodic arrangement — model as spin degrees of freedom residing on lattice sites

d-dimensional lattice; sites $i = 1 .. N$

examples:
- 3d cubic lattice  coordination number $z = 6$
- 2d cubic lattice (square lattice)  coordination number $z = 4$
- 2d triangular lattice  coordination number $z = 6$.

Site i: quantum-mechanical spin $\vec{S}_i = (S_{ix}, S_{iy}, S_{iz})$ (operator)

(e.g., spin-$\frac{1}{2}$: $\vec{S}_i = \frac{1}{2}\hat{\vec{\sigma}}_i$)

Interacting spin model

$$\hat{H} = -\sum_{\underset{\uparrow}{\langle ij \rangle}} J\, \vec{S}_i \cdot \vec{S}_j \quad \underbrace{- \vec{H}_{ext} \cdot \sum_i \vec{S}_i}_{\text{Zeeman energy of spins in external field}}$$

nearest neighbour bonds

Heisenberg model; full quantum formulation

With the above convention, $H = \ldots - J \vec{S}_i \cdot \vec{S}_j \ldots$

$J > 0$ - ferromagnetic coupling (wants spins to be parallel, $\uparrow\uparrow$)

$J < 0$ - antiferromagnetic coupling (wants spins to be antiparallel) $\uparrow\downarrow$

Deformations of the Heisenberg model: $\vec{S}_i \cdot \vec{S}_j = \underbrace{S_i^x S_j^x}_{\times J_x} + \underbrace{S_i^y S_j^y}_{\times J_y} + \underbrace{S_i^z S_j^z}_{\times J_z}$

"Easy axis" spins: sometimes lattice environment is such that the x-x and y-y couplings are smaller than the z-z couplings. In the limit $J^x = J^y = 0$, obtain Ising model

$$H = -\sum_{\langle ij \rangle} J S_i^z S_j^z - H_{ext} \sum S_i^z$$

imagine oriented along the easy axis.

Hamiltonian is diagonal in the S^z-basis, so know all eigenstates & eigenenergies

$$E[\{S_i^z\}] = -\sum_{\langle ij \rangle} J S_i^z S_j^z - H \sum S_i^z$$

$$\underset{e^{-\beta H}}{Tr\{\ldots\}} = \sum_{\{S_i^z\}} e^{-\beta E[\{S_i^z\}]}$$

"classical" statistical mechanics problem

Spin-$\frac{1}{2}$: $S_i^z = \pm\frac{1}{2}$. Often Ising model is defined with $S_i = \pm 1$ (simple rescaling of J)

Classical Ising model - challenging interacting stat. mech problem.

⊛ "Easy-plane" spins : if $J^x = J^y > J^z$
e.g., with $J^z = 0$

$$H = -J \sum_{\langle ij\rangle} \underbrace{(S_i^x S_j^x + S_i^y S_j^y)}_{\text{only in the } x-y \text{ plane}}$$

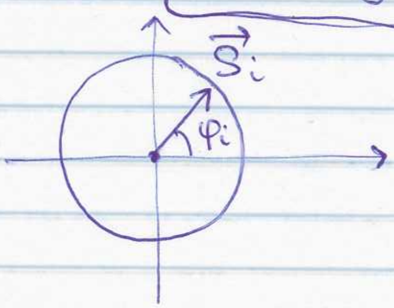
} complex quantum-mech. problem where we cannot find eigenstates

At finite temperature, $\vec{S_i} = (S_{ix}, S_{iy})$ behaves like a "classical" vector

$$\mathrm{Tr}\{\ \} \approx \int \prod_i d\vec{S_i}\, \delta(\vec{S_i}^2 = 1)\ \{\ldots\}$$

Classical XY model

$$\boxed{Z = \int \prod_i d\vec{S_i}\, \delta(S_{ix}^2 + S_{iy}^2 = 1)\ e^{-\beta E(\{\vec{S_i}\})}}$$



- can be also formulated in terms of "angles" $\phi_i \in (0, 2\pi)$

$$\vec{S_i} = (\cos\phi_i, \sin\phi_i)$$

Measure $\displaystyle \int d\vec{S_i}\, \delta(S_{ix}^2 + S_{iy}^2 = 1) = \int_0^{2\pi} d\phi_i$

interaction

$$-J\vec{S_i}\cdot\vec{S_j} = -J\cos(\phi_i - \phi_j)$$

$$\boxed{Z = \int_0^{2\pi} \prod d\phi_i\ \exp\Big(\beta J \sum_{\langle ij\rangle} \cos(\phi_i - \phi_j)\Big)}$$

Besides easy-plane magnets, this model is also used to describe normal to superfluid transition in He^4
(roughly, "order parameter" ~ complex wavefnctn
ϕ ~ phase of the order parameter)

(O(n) model)

$\circledast$ Classical
<u>n-vector model</u> $\vec{S}_i = (S_{i1}, S_{i2}, \dots, S_{in})$ – unit n-dim. vector, $\vec{S}_i^{\,2} = 1$

$$E[\{\vec{S}_i\}] = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$n=1$ – Ising model
$n=2$ – classical XY model
$n=3$ – Heisenberg model (O(3) model)
classical

$n=\infty$ – "spherical model"

<u>Exactly soluble</u>:
- $n=\infty$ in any dimension d
- Ising model in $d=1$ (simple)
  $d=2$ (highly nontrivial)

<u>Qualitatively soluble</u>: all models in $d \geq 4$, in the sense that meanfield treatment gives exact critical exponents.

<u>Magnetically ordered phase</u> (ferromagnet) (for $J>0$ and low temperature)

Aside: When discussing non-interacting systems (ideal gas; Fermi gas; non-interacting spins), with the exception of BEC, we were studying properties of one phase which is continuously connected to high temperatures.

Start the lecture here:

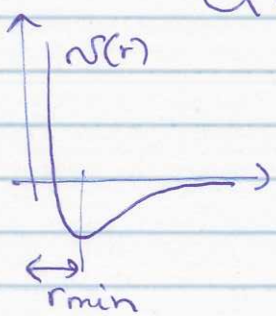
In the interacting classical gas, we have encountered interaction giving rise to denser liquid phase coexisting (long-range attraction) with less dense gas phase (liquid-gas transition); but liquid is not distinct from gas

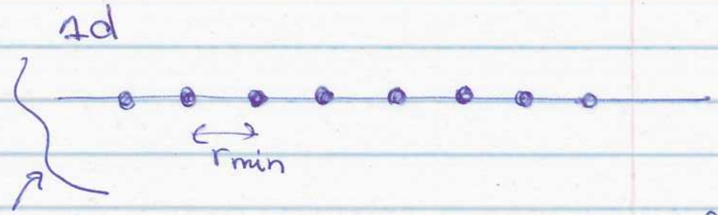
More generally, interactions give rise to new phases ("states of matter") at low temperature, not connected to the high-temperature.

Schematically, at low temperatures entropic effects are not important and the system tries to minimize the interaction energy. Very often, minima of the interaction energy have some order breaking some symmetries of the system.

<u>example</u>: crystaline order of clasically interacting particles

$$U(\{\vec{q}_i\}) = \sum_{\langle ij\rangle} v(q_i - q_j)$$





can imagine this being the global minimum

(e.g., $\frac{\partial U}{\partial q_i} = 0$ – "no force"

$\frac{\partial^2 U}{\partial q_i^2} > 0$ – minimum of energy)

$U(\{q_i\})$ is invariant under translations,

$q_i \to q_i + a$ with arbitrary a

The classical ground state is not invariant – broken translational symmetry.

Instead, translations by $a \neq (\text{int}) \cdot r_{min}$ give non-equivalent (but energetically degenerate) ground states.

Back to magnetic systems – these provide excellent example of "ordered phases" at low temperature due to interactions.

- At high temperature $(T \to \infty)$, entropic effects dominate ($F = U - TS$ – to minimize F want to have large S)

→ spins are essentially randomly oriented ("paramagnet")

(Can improve on this "completely randomized spins" picture by using perturbative treatment in J/T, as in one of the HW problems)

- At $T=0$, want to minimize $E[\{\vec{S}_i\}]$.
For $J>0$ (ferromagnetic interaction), the minimum is "all spins parallel"

$$\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$$

* For Ising spins, two energetically equivalent ground states are $\{\text{all } S_i=+1\}$ or $\{\text{all } S_i=-1\}$. The system "freezes" into one or the other depending on the history. Either state breaks the Ising symmetry of the model: $S_i \to -S_i$
(formally $E[\{S_i=-S_i'\}] = E[\{S_i'\}]$)

* For $O(n\geq 2)$ spins, there is a continuum of degenerate ground states

$$\uparrow\uparrow\uparrow\uparrow\uparrow \quad \text{or} \quad \nearrow\nearrow\nearrow\nearrow\nearrow \quad \text{or} \quad \downarrow\downarrow\downarrow\downarrow\downarrow$$

Each state breaks continuum symmetry $\vec{S}_i \to R_n \vec{S}_i$

$$(R_n\vec{S}_i)\cdot(R_n\vec{S}_j) = \vec{S}_i\cdot\vec{S}_j$$

R_n: $O(n)$ rotation (same for all sites)

- Expect that there exists T_c s.t. the system is
  - paramagnet for $T>T_c$
  - ferromagnet for $T<T_c$

T_c – transition temperature

Quite generally

* $T_c\uparrow$ if $d\uparrow$ or $z\uparrow$ (more "bonds" must be broken to destroy the magnetically ordered state)

* $T_c \downarrow$ if $n \uparrow$ in the n-vector model
(number of "available states" goes up)

Example:

	Ising	XY	O(3) Heisenberg
d=2	$T_c > 0$	no true LRO, only QLRO	$T_c = 0$
d=3	$T_{c\,Ising} > T_{c\,XY} > T_{c\,O(3)}$ (for fixed J)		

* $T_c \downarrow$ if replace classical spin by quantum-mechanical spin (q.m. spin has "more states available" - "q.m. fluctuations")
because of non-commutation of S_x, S_y, S_z

Other interpretations of lattice models

1) Ising model $\leftrightarrow$ lattice gas

$$S_i = \{+1, -1\} \leftrightarrow n_i = \frac{S_i+1}{2} = \{\underset{\text{occupied}}{1}, \underset{\text{empty}}{0}\}$$

$$-J_{ij} S_i S_j = -J_{ij}(2n_i - 1)(2n_j - 1) =$$

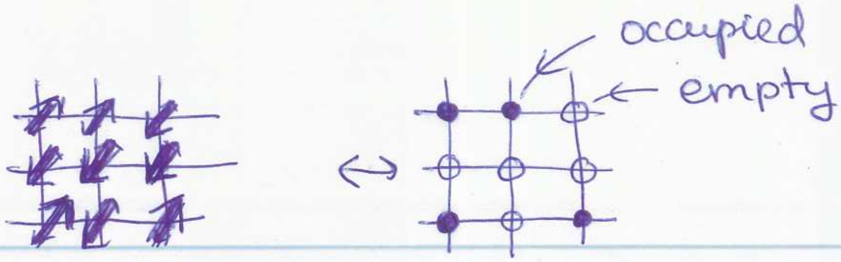
$$= \underbrace{-4J_{ij} n_i n_j}_{\substack{\text{density-density}\\ \text{interaction}}} + \underbrace{2J_{ij}(n_i + n_j)}_{\substack{\text{Contrib.}\\ \text{to "chemical}\\ \text{potential"}}} - \underbrace{J_{ij}}_{\text{const}}$$

$$H = -J\sum_{\langle ij \rangle} S_i S_j - h\sum_i S_i = \sum_{\langle ij \rangle} V_{ij} n_i n_j - \mu \sum_i n_i + \text{const}$$

$$V_{ij} = -4J_{ij}$$

J ferromagnetic $\leftrightarrow$ $V < 0$ - attractive interaction
$J > 0$

$m = M/\text{Vol} \leftrightarrow \frac{2N}{\text{Vol}} - 1 = 2n - 1$ (n: density per site)



kinetic energy is neglected, but molecules interact:

potential energy of 2 particles @ locations i & j $= \begin{cases} +\infty & \text{if } i=j \\ \varepsilon_0 = -4J & \text{if } i \,\&\, j \text{ are nearest neighbours} \\ 0 & \text{otherwise} \end{cases}$

Ising problem in the field h $\leftrightarrow$ lattice gas problem at fixed chemical potential

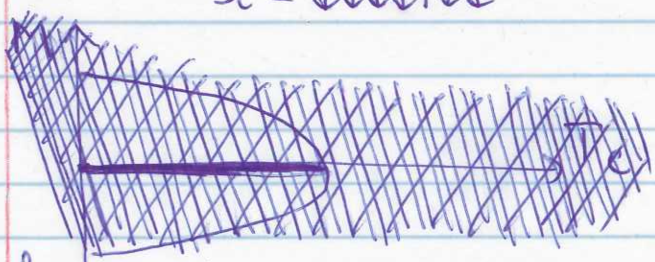
For $T < T_c$

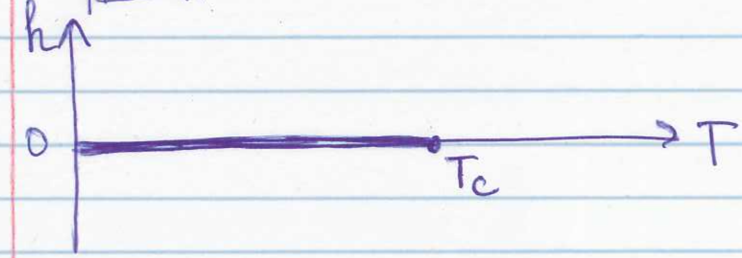
$h>0$, spins predominantly $\uparrow$ $\leftrightarrow$ high density phase ("liquid")

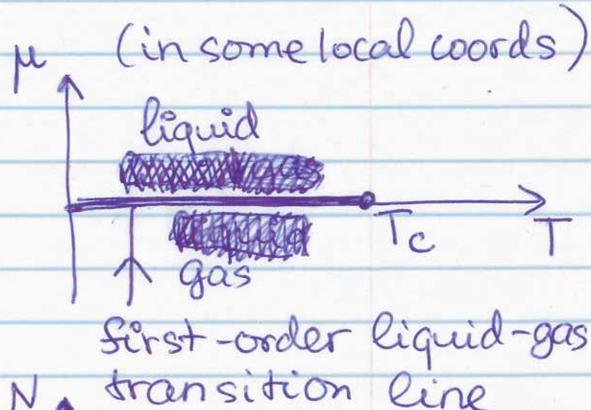
$S_i = \uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow$ $\quad n_i = 1110111$

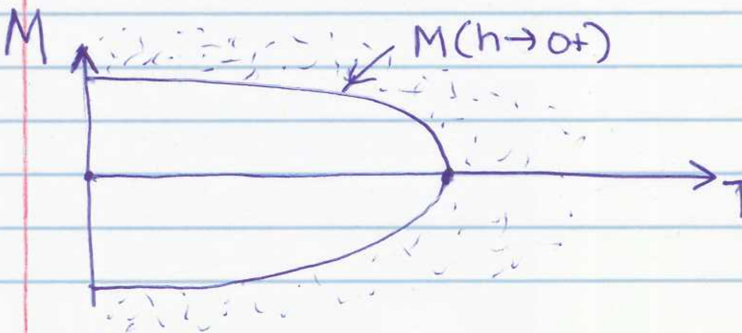
$h<0$, spins predominantly $\downarrow$ $\leftrightarrow$ low density phase ("gas")

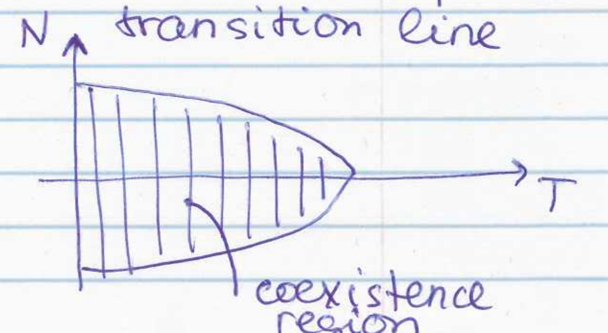
$S_i = \downarrow\downarrow\downarrow\downarrow\uparrow\downarrow\downarrow$ $\quad n_i = 0000100$



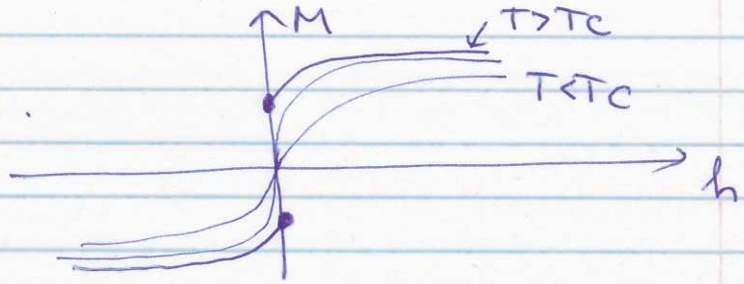






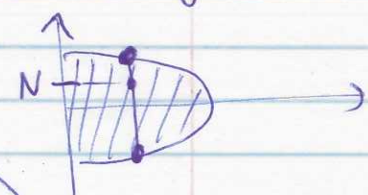


Mathematically the two problems are identical. The difference is only in typical experimental settings: for magnetic systems, one typically controls h and measures M.

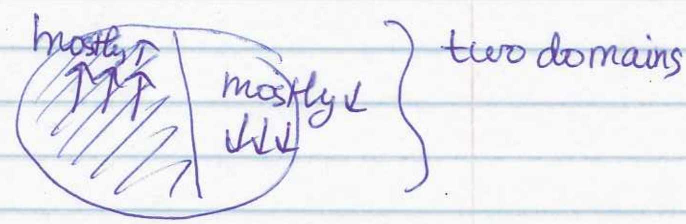


For particles systems, one is more likely to control N.

Example: liquid-gas coexistence at fixed N



Magnet at fixed M



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2) Ising model $\longleftrightarrow$ binary alloy

$n_i = 0 \Leftrightarrow$ occupied by A-type

$\phantom{n_i = {}}1 \quad$ occupied by B-type

3) XY model $\longleftrightarrow$ superfluid ^4He