UNIVERSITY OF TEXAS ARLINGTON

PHYS 5319-001: Math Methods in Physics III

Monte Carlo Simulation on Ising Model

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Statistical Mechanics (recap)

- Study the overall behavior of a system of many particles.
- A macroscopic state: *V, T, P, magnetization (M), etc.*
- A microscopic state: $\{\vec{r}_i, \vec{p}_i\}$ $(i = 1,2, \ldots, N)$

  a point in Γ-space, changing with time
- 1 macro state $\longrightarrow$ huge number of microscopic states
- Ensemble: a collection of all these microscopic states
- All the macro (measurable) physics quantities came from the ensemble average.

$$\langle A \rangle = \sum_\alpha A_\alpha P_\alpha$$

$$\langle A \rangle_t = \frac{1}{\tau}\int_0^\tau A(t)dt$$

where P_α: probability for microstate α

More Stat Mech recap

- different ensembles ↔ different macro restrictions
- Canonical ensemble: constant (*N*, *V*, *T*)

if the total energy of the system is E_α for α–th state/configuration,

$$P_\alpha \sim e^{-E_\alpha/kT}$$

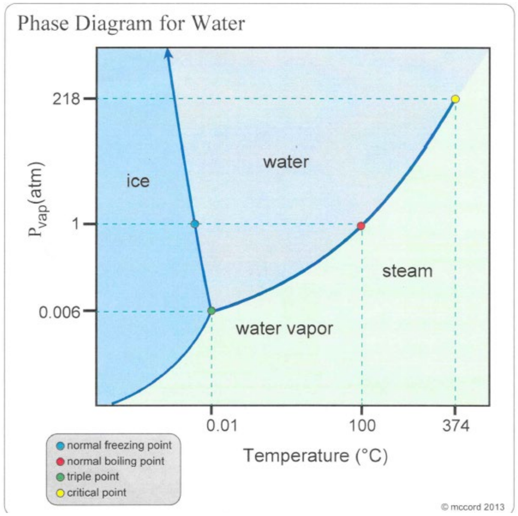
where *k* is Boltzmann constant

- So, all the microscopic states has contributions.
- Partition function $Q_N = \sum_\alpha e^{-E_\alpha/kT} \Rightarrow$ macro properties
- But Q_N is hard to obtained unless the inter-particle interaction is negligible: $E_\alpha = \sum_i \varepsilon_i$

$$Q_N = \frac{1}{N!} Q_1^N$$

where $Q_1 = \sum_n e^{-\varepsilon_1(n)/kT}$ $\qquad$ n: single particle state

Phase & phase transition

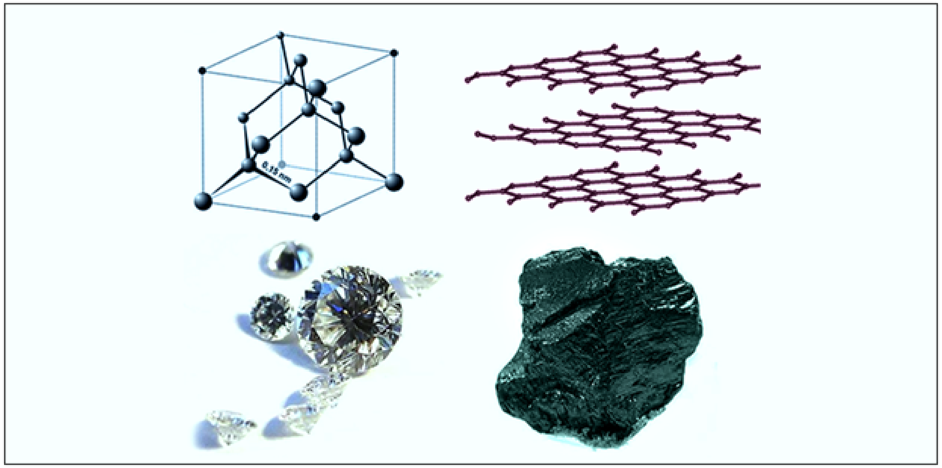


- Phase: a physically distinctive form of a substance

  e.g. solid, liquid, gas, plasma
- Phase transition: a transformation from one to another

  at $T=T_c$
- Different phases for a solid carbon:

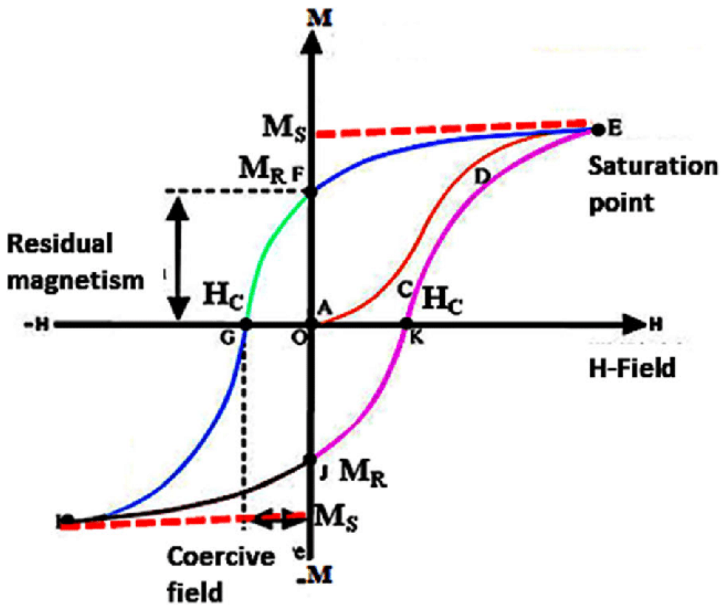
diamond & graphite

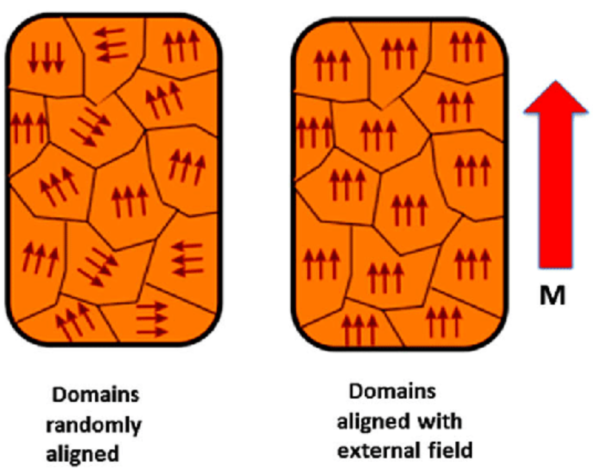


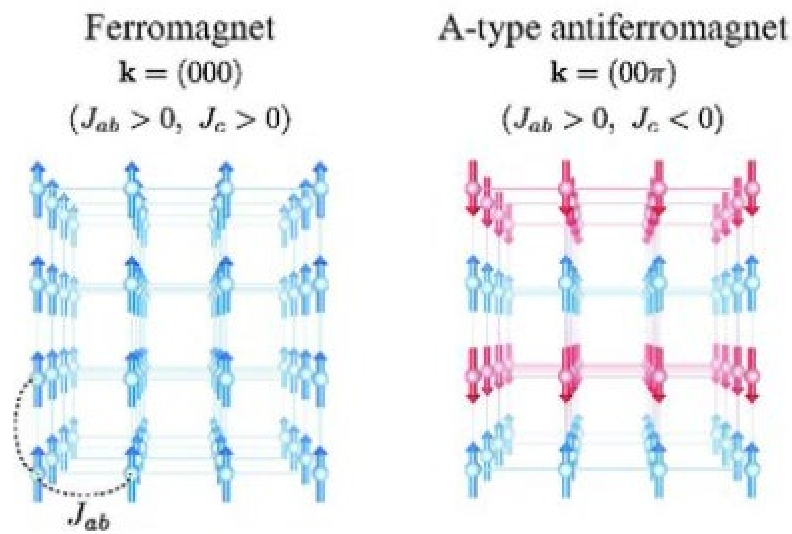
- Magnetic ordering of matter:

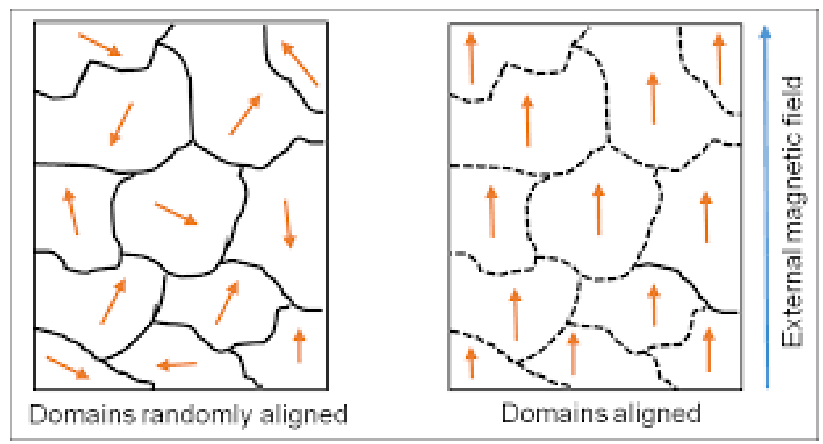
  paramagnetic, ferromagnetic, antiferromagnetic

Magnetic Ordering









$2^{10} = 1024$

Ising Model

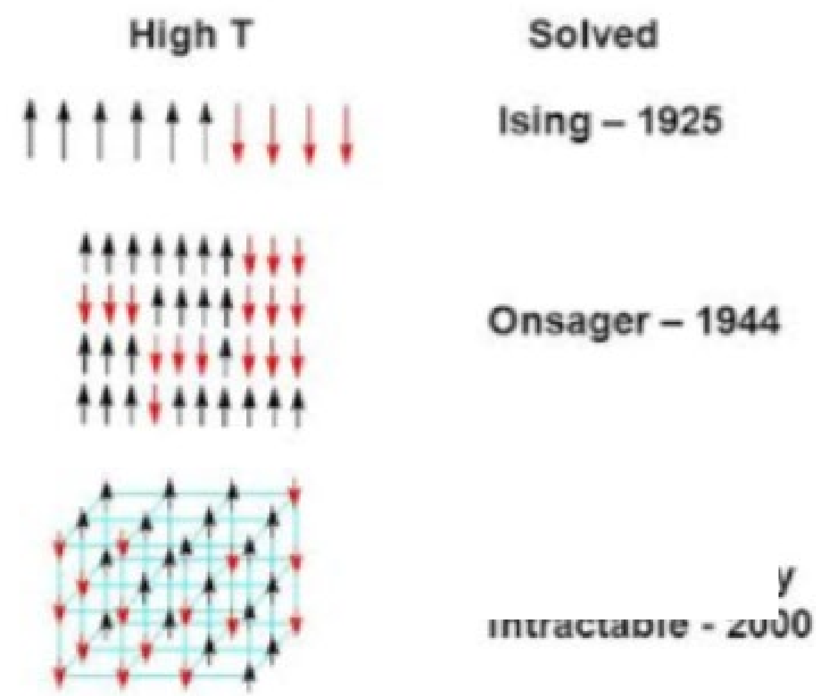
$U = -\vec{\mu}\cdot\vec{H}$

$= \pm \mu H$

An array of N magnetic dipoles ("spins") on fixed points (lattice) in a uniform magnetic field H.

$$E_I\{s_i\} = -\sum_{<ij>} J_{ij} s_i s_j - H \sum_{i=1}^{N} s_i$$

S_i=1 or -1 (up or down); <ij> only consider the nearest neighbor; J_{ij} *(>0)* is the coupling constants.



For a system of N spins ($N \to \infty$), each spin configuration is a micro-state (α).

probability $P_\alpha \sim e^{-E_\alpha/kT}$

A macroscopic measurement $\langle A\rangle = \sum_\alpha A_\alpha P_\alpha$ e.g. $M = \sum_\alpha M_\alpha P_\alpha$

But, how many α? 2^N

Mean field theory

- Each spin (moment μ) is in a “smeared-out” (mean field) environment.

  i.e. $M = \sum_i \langle S_i \rangle = N \langle S \rangle$

- In an external magnetic field ($H=B/\mu_0$): $E = -J\sum_{<ij>} S_i S_j - \mu H \sum_i S_i$

  or $E = \sum_i \{ -\underline{(J\sum_{j\neq i} S_i)} S_j - \mu H S_i \} = \sum_i \varepsilon_i$

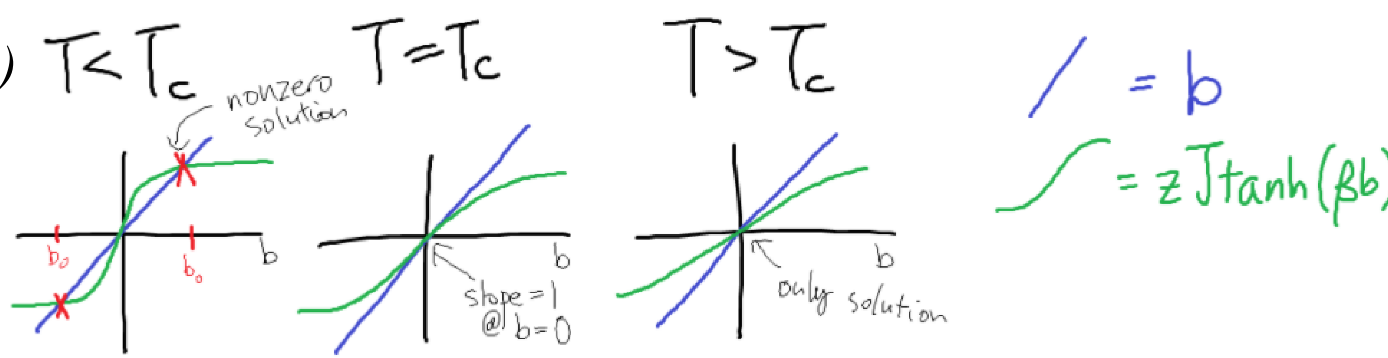
  Like an effective field $H_{eff} = \frac{J}{\mu}\sum\langle S\rangle = \frac{zJ}{\mu}\langle S\rangle$

- Now $H + H_{eff} \rightarrow H'$. For $S_i = \pm 1, \varepsilon_i = \varepsilon_\pm = \mp\mu H'$
- $Q_1 = \sum_i e^{-\varepsilon_i/kT} = e^{\mu H'/kT} + e^{-\mu H'/kT}$ ⇒ probability $p_\pm = e^{\mp\mu H'/kT}/Q_1$

  $\langle S\rangle = \sum_i S_i p_i = p_+ - p_- = tanh(\mu H'/kT)$ recall $H' = H + \frac{zJ}{\mu}\langle S\rangle$

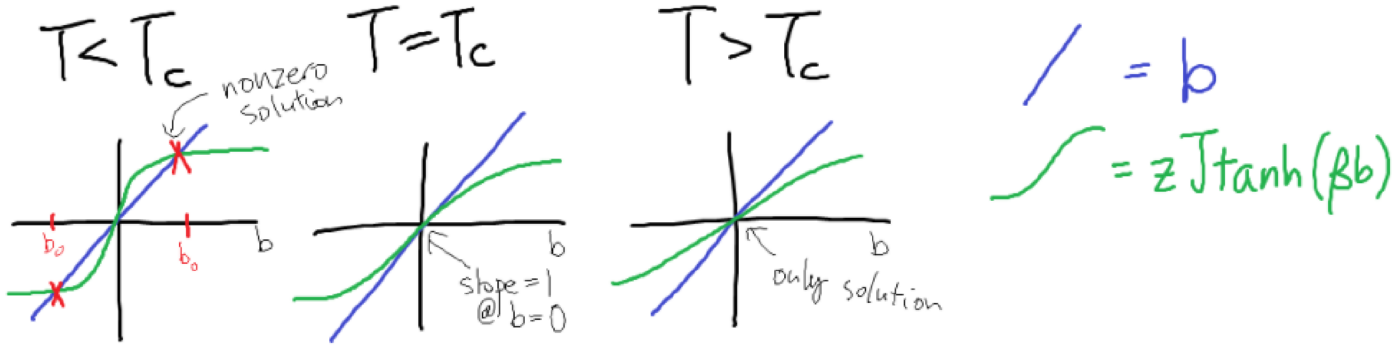
- So, we have an equation $\underline{\langle S\rangle} = tanh(\frac{H}{kT} + \frac{zJ}{kT}\underline{\langle S\rangle})$ *no analytic solution*
- Graphical solution

  (For external H=0)



$$\langle S\rangle = -s_0, 0, s_0$$

$$T_c = \frac{k}{zJ}$$

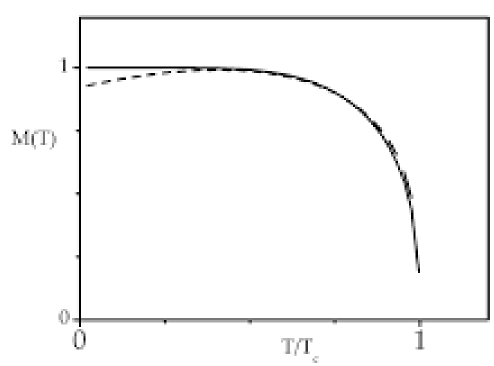


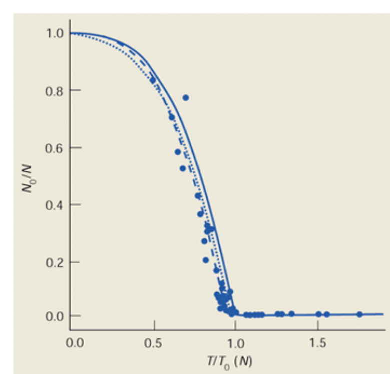
$\langle S \rangle = -s_0, 0, s_0$

Since M=N<S>, we have

$M > 0 \quad at\ T < T_c$
$M = 0 \quad at\ T > T_c$

In general, $M \propto (T - T_c)^{\beta}$ β: critical exponent





Bose-Einstein Condensation