Note Title 18-04-2019

Monte Carlo Simulations / ISING MODEL.

Phase Transitions. → FERROMAGNETIC – PARAMAGNETIC PHASE TRANSITION AS TEMP ↑ (increases)

SIMULATIONS → $\underset{\smile}{?}$ Modeling a physical system on the computer.

Position / Velocities & Hamiltonian (p_N, q_N)

or appropriate degrees of freedom.

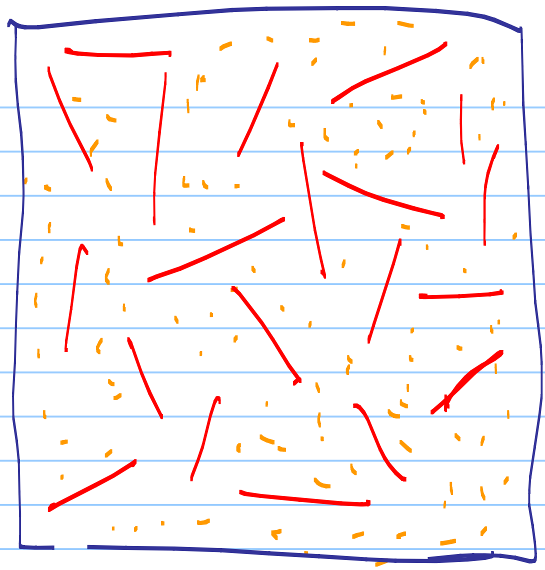
STATISTICAL Physics → Calculate thermodynamic properties of the system
(From microscopic physics)

Monte Carlo : Stochastic Methods → Random no. generator

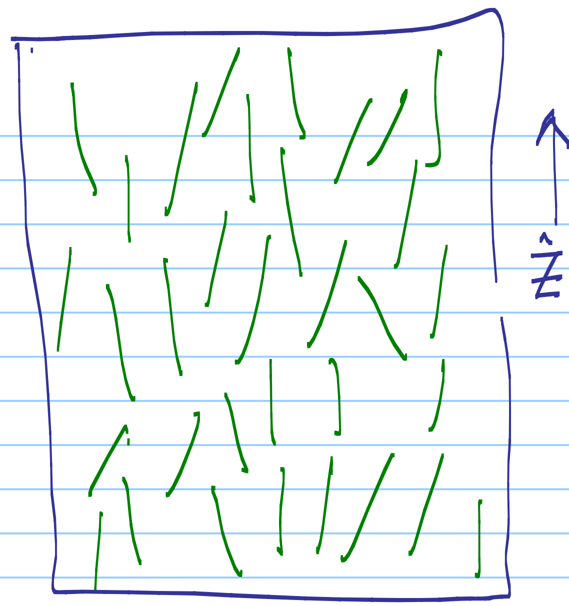
Ising Model : using a Model Hamiltonian → magnetic properties.

Phase Transition.

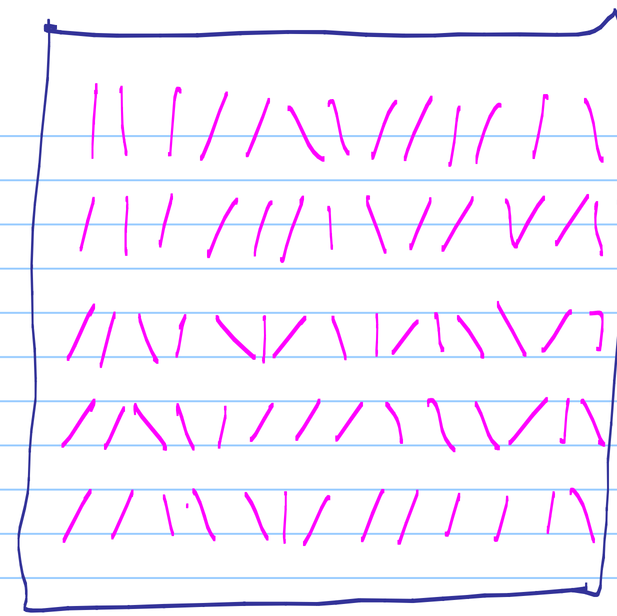
1. Solid → Liquid → Gas.
2. Ferromagnetic → No net Magnetic moment
   Disordered state at high temp T.
3. Superconducting Phase Transition.
4. LIQUID CRYSTALS
   (ISOTROPIC → NEMATIC → SMECTIC)



Disordered

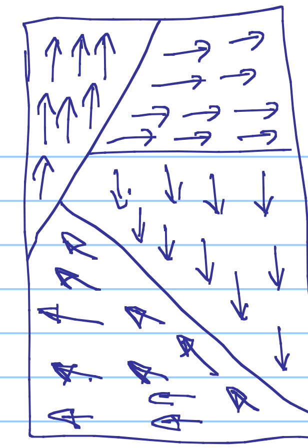


Nematic State



Smectic State

5. Napolean's Russian War in Winter.

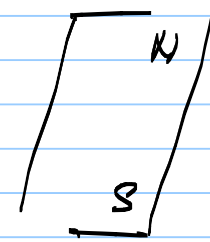


β – TIN $\longrightarrow$ α – TIN.

(ductile/metallic) (powdery phase).

Ferromagnetic Transitions.

Iron	Cobalt	Nickel
1043 K	1388 K	627K.
770°C	1115°C	354°C

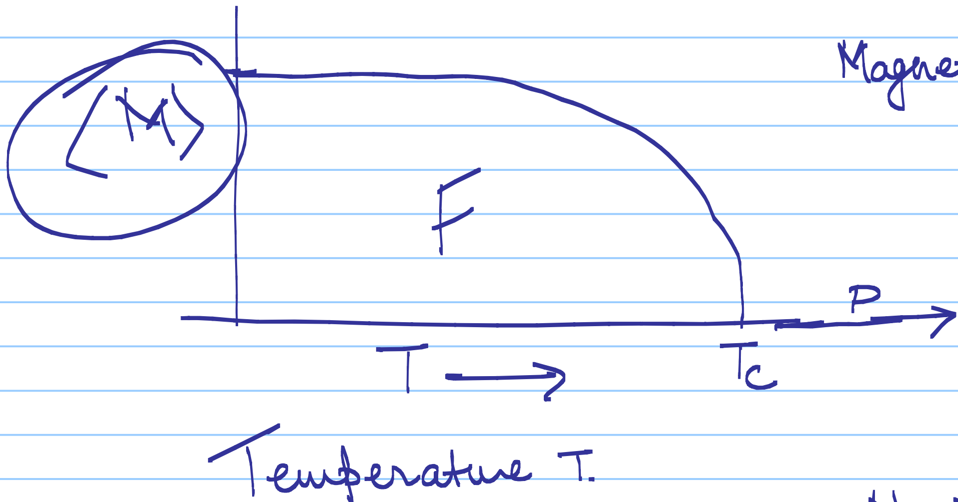


Bar Magnet.

Paramagnetic State $\not\rightrightarrows$ PARAMAGNET.

Concept of an ORDER Parameter (?).

Order parameter : Quantity (Calculated / Measured) which can be used to distinguish between 2 phases or states.



Magnetic feild $B = 0$.

$\langle M \rangle \rightarrow$ Magnetization (Order parameter)

$\langle M \rangle / N$ per spin

$N \rightarrow$ total no. of spins in the System

KIND OF PHASE TRANSTIONS (1st ORDER vs 2nd Order)

THERMODYNAMIC QUANTITIES which are obtained from first order

1st order phase Transition : derivatives of free energy F (or G) show a DISCONTINUITY

(Energy E, Magnetization M, volume per particle)

2nd order Phase Transition : 2nd order derivatives of F (or G) show a singularity.

heat capacity $\rightarrow C_V$, χ , κ (Compressibility)

$\chi \rightarrow$ magnetic susceptibility.

(STAT-MECH REMINDERS)

$$\langle E \rangle = \frac{\partial}{\partial \beta}(\beta F) \qquad \beta = \frac{1}{k_B T}$$

$k_B \rightarrow$ Boltzman const. $= R/N_A$

$$\langle E \rangle = U = -T^2 \frac{\partial}{\partial T}(F/T)_{V,N}$$

$\rightarrow$ first derivative

$$\langle M \rangle = -\frac{\partial F}{\partial B}\Big|_{N,T}$$

$$C_V = \frac{\partial U}{\partial T}\Big|_{V,N} \qquad \chi = \frac{\partial \langle M \rangle}{\partial B}\Big|_{T,N}$$

$$Z = \sum_i e^{-\beta E_i} \quad \text{(partition fn).}$$

(sum over all microstates).

$E_i \rightarrow$ energy of a microstate.

$$F = -k_B T \ln Z$$

Average energy of a system <u>CANONICAL ENSEMLE</u>

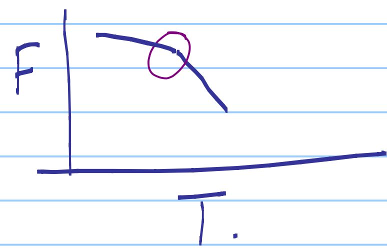
$$\langle E \rangle = \sum_i \frac{E_i e^{-\beta E_i}}{Z}$$

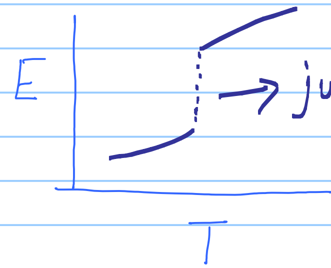
$$= \frac{1}{Z}\sum -\frac{\partial}{\partial \beta} e^{-\beta E_i} = -\frac{1}{Z}\frac{\partial}{\partial \beta}\overbrace{\sum_i e^{-\beta E_i}}^{Z}$$

$$= -\frac{1}{Z}\frac{\partial}{\partial \beta} Z = -\frac{\partial}{\partial \beta}(\ln Z) = \frac{\partial}{\partial \beta}(\beta F).$$

So

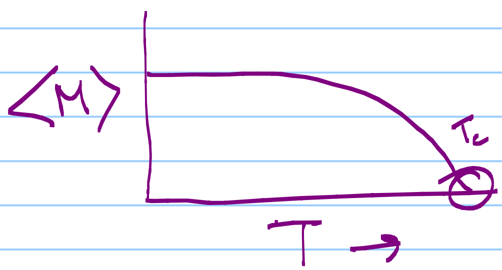
In First Order Transition $\langle E \rangle$ would show a jump.

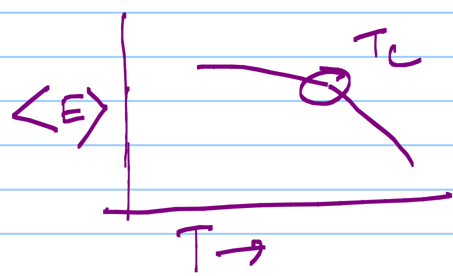


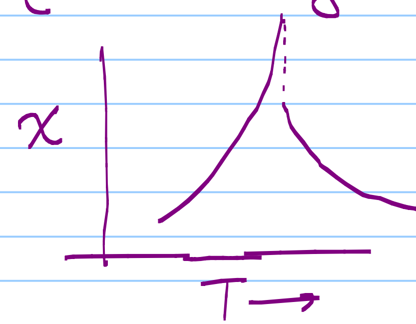


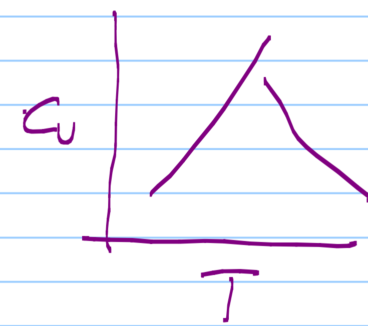
→ jump → Latent heat.

In 2nd Order Phase Transition (Ferromagnetic Transition)

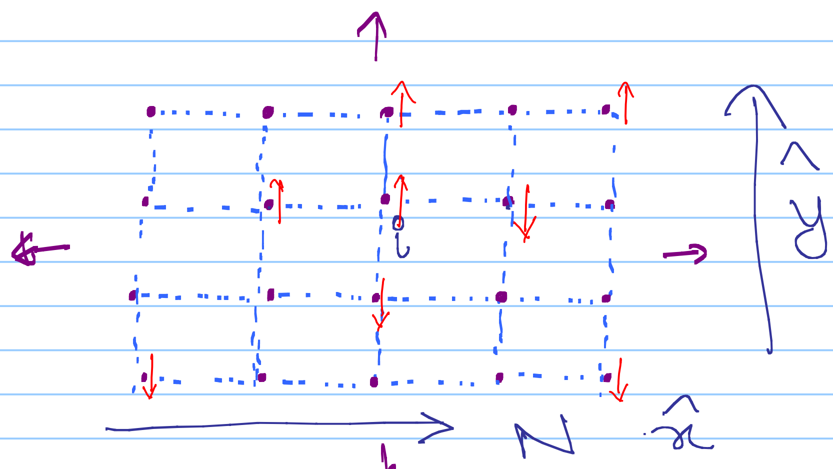






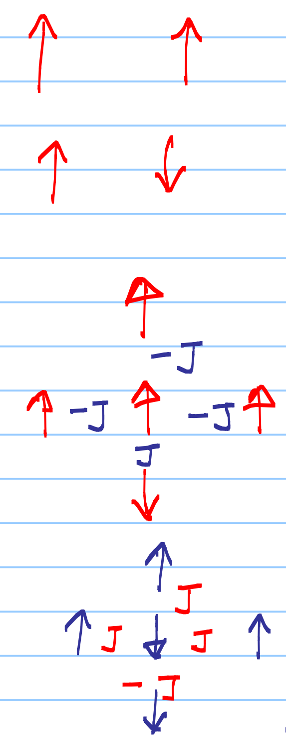


ISING MODEL → MODELS THE FERROMAGNET.



$$\mathcal{H} = -J \sum_{\substack{i=1 \\ j=1,2,3,4}}^{N^2} S_i S_j + H_{KE} + H_{LATTIC}$$

(over neighbour of spin i).



Energy = $-J . \times 1 \times 1$.

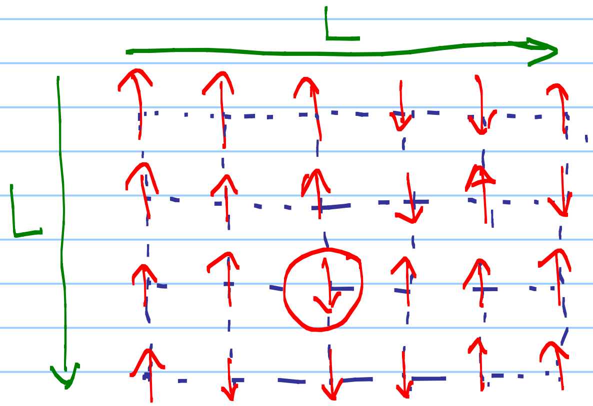
Energy = $-J \times -1 \times 1$
$= J$

Energy = $-2J$.

Energy = $2J$

$\Delta E = 2J - (-2J) = 4J$

HOW TO SIMULATE THE ISING MODEL. (ALGORITHM)



→ GENERATE DIFFERENT MICROSTATE

↓ HOW ?

→ CHOOSE A RANDOM SPIN.

→ CALCULATE E_1 (INTERACTION ENERGY WITH NEIGHBOURS)

$$\Delta E = E_2 - E_1$$

→ GIVE A TRIAL FLIP → CALCULATE E_2

→ IF $\Delta E \leq 0$ THEN ACCEPT SPIN FLIP

→ IF $\Delta E > 0$ THEN ACCEPT SPIN FLIP WITH Prob $e^{-\Delta E / k_B T}$.

→ DO THIS ATTEMPT FOR ALL THE SPINS.

→ N = Total No. of spins = $L \times L$ spins.

→ N attempts to flip the spins → 1 Monte Carlo Step → MCS.

→ Only some spin flip attempts will be sucessful.

→ Depends on the value of $k_B T$. (thermal Energy).

→ $$\begin{array}{ccc} & \uparrow & \\ \uparrow & \uparrow & \uparrow \\ & \downarrow & \end{array} \Longrightarrow \begin{array}{ccc} & \uparrow & \\ \uparrow & \downarrow & \uparrow \\ & \downarrow & \end{array} \qquad \Delta E = 2J - (-2J) = 4J.$$

E_1 $-J-J-J+J = -2J$ $\qquad$ $E_2 = +J+J+J-J = 2J$

ΔE is (+)ive → Flip with Probability e^{-4J/k_BT}

→ ENERGY OF THE MICROSTATE INCREASES !

$e^{0/k_BT} = 1.$

$e^{-4J/k_BT} < 1$

WHERE IS THIS EXCESS ENERGY COMING FROM?

THERMAL RESERVOIR → CANONICAL ENSEMBLE

NOT explicitly modeled

→ Energy exchange with reservoir → Statistical Mechanics.

→ Do MANY Monte Carlo Steps → System Relaxes to Equilibrium (Independent of the Initial configuration).

→ Remember. Equilibrium ≡ COLLECTION OF MICROSTATES.

$$P(\epsilon_i) = \frac{e^{-\epsilon_i/k_B T}}{Z}$$

BIASED SAMPLING.

→ When chosing spin for TRIAL FLIP → one has to RANDOMLY choose a spin to flip.

How To Implement All This On The Computer?

ARRAY : Spin (L, L). $L = 20$ spin $(20, 20)$.

INITIALIZE : spin $(1,1) = 1$ spin $(1,2) = 1$ spin $(2,3) = -1$

RANDOM INITIAL CONDITION OR.
ALL SPINS UP(+1) OR ALL SPINS DOWN (−1).

MONTE CARLO ALGORITHM (IN DETAILS)

BROAD FLOWCHART → ① INITIALIZE LATTICE.

② EQUILIBRATION AT A PARTICULAR T

③ GENERATE MICROSTATES AT A PARTICULAR T.

N_{MCS} → CANONICAL ENSEMBLE

④ CALCULATE THERMODYNAMIC QUANTITIES.

$\langle E \rangle, \langle M \rangle, \langle C_v \rangle, \langle \chi \rangle.$

$$\langle E \rangle = \sum_k E_i \frac{e^{-\beta E_i}}{\boxed{Z}}$$

SO $\equiv \langle E \rangle = \frac{\sum E_i}{N_{MCS}}$

BIASED MONTE CARLO

BUT METROPOLIS ALGO ACCESSES STATES WITH PROB $e^{-\beta E_i}/Z$

⑤ CHANGE TEMPERATURE T

⑥ PLOT AND MONITOR $\langle \ \rangle$ QUATITIES WITH T.

→ DO PHYSICS.

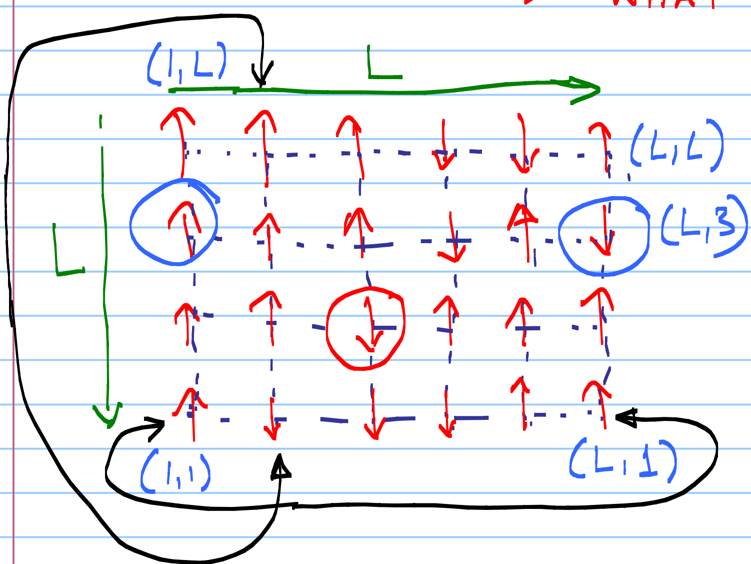
QUESTIONS

→ HOW DO WE KNOW HOW SYSTEM IS IN EQUILIBRIUM?

→ HOW DO WE KNOW THAT THE THERMODYAMIC AV. $\langle \ \rangle$ IS GOOD ENOUGH AND RELIABLE?

→ WHAT ABOUT FINITE SIZE EFFECTS?

spin(i,j)



BOUNDARY EFFECTS

↓ PBC

(PERIODIC BOUNDARY CONDTIONS)

SMALL SIZE OF LATTICE $\ll N_{AV}$

$(i-1,j)$ $\quad$ (i,j) $\quad$ $(i+1,j)$

$(i,j-1)$

BUT

NEIGHBOUR OF

$(L,3) \rightarrow (1,3)$

$(2,1) \rightarrow (2,L)$

UNITS.

MAGNETIC MOMENT $\vec{\mu} \Rightarrow \mu_B S_i$

Bohr Magneton

spin $S \to$ angular momentum $\to \hbar \to \pm 1$.

MAGNETIZATION

$\longrightarrow$ ORDER PARAMETER $\to \langle M \rangle / \langle M_{max} \rangle \equiv \dfrac{\langle \sum S_i \rangle}{S_{MAX}} = \langle O \rangle = \langle M \rangle$.

AT LOW $T \to \langle O \rangle \equiv \langle M \rangle = 1$.
(AT $T=0$)

AT HIGH $T \longrightarrow \langle M \rangle = 0$.

$$\mathcal{H} = -J \sum_{i=1}^{N=L\times L} S_i S_j$$

$j = 1,2,3,4$ (in SQUARE LATTICE).

UNITS OF ENERGY

$$\langle E \rangle = \left\langle -J \sum S_i S_j \right\rangle$$

QUANTUM MECHANICAL CALC (eV).

OTHER UNIT OF ENERGY IS $K_B T$.

k_B = Boltzmann's Constant $= \frac{R}{N_A} = \frac{8.32}{6.02 \times 10^{23}}$ (SI units)

$= 1.38 \times 10^{-23}$

$eV = 1.6 \times 10^{-19}$ Joules.

$1\,eV = \frac{1.6 \times 10^{-19}}{4.2 \times 10^{-21}} \simeq 0.38 \times 10^{2}$

4.2×10^{-21} ($K_B T$ at ROOM TEMP) $K_B T_{300}$

$K_B T$ (at $T = 300K$) $= 3 \times 1.4 \times 10^{-21}$

$= 4.2 \times 10^{-21}$ Joules.

$\hookrightarrow \langle K.E \text{ per particle} \rangle = \frac{3}{2} K_B T$

AT WHAT T VALUE IS $K_B T = 1.6 \times 10^{-19}$ J.

$$T = \frac{1.6 \times 10^{-19}}{1.38 \times 10^{-23}} = 1.16 \times 10^{4} \simeq 11{,}000\,K.$$

WE MEASURE T ($K_B T$) in UNITS OF J

SET $J = 0.05\,eV$ (SAY) $\longrightarrow$ $J = 1$.

$0 \cdot 1\, eV = 2J.$

$0 \cdot 3\, eV = 6J.$

Similarly measure $K_B T$ in units of J

$K_B T = 2J, \quad 0 \cdot 2J, \; 5J$ and so on.

If $K_B T = 2J \longrightarrow K_B T = 0 \cdot 1 eV$

$\rightarrow T = 0 \cdot 1 eV / K_B.$

Lets LOOK AT ACTUAL CODE.