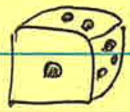
Take picture of board.

Probability

01/11/2025.

1. • Definitions.

9:30–9:35 ① 

$\Omega = \{1, 2, 3, \cdots, 6\}$: sample space.

$E = \{1\}, \{2,4\}, \cdots$: event.

② 

$\Omega = \{ r \mid 0 \leq r \leq r_{max} \}$: sample space

$E = \{ r^{(1)} = 0.23 \}, \ldots$: event.

$\{ r^{(1)} = 0.1,\ r^{(2)} = 0.2 \}$

→ Probability : Event / Sample space.

1) Objective probabilities

$p = \lim_{N \to \infty} \frac{N_E}{N}$

2) Subjective probabilities.

Theoretical estimate. ~ 1/6 dice.

Q) Monty Hall problem.

$\boxed{1}$	$\boxed{2}$	$\boxed{3}$	Result (stay #1)	Result (change to offered)
G	G	C	G	C
G	C	G	G	C
C	G	G	C	G.
			→ 1/3	→ 2/3

Rule : Host must,

1) open door not selected by contestant.

2) open door to reveal goat not car.

3) offer chance to switch btw original and remaining closed.

2. • Q) : 20 people at least two have same birthday

9:35–9:40

$$P = 1 - \frac{{}_{365}P_{20}}{365^{20}} \approx 0.4114.$$

3. • Rules. (in HW)

9:40–9:45

- *Additive* : $P(A \cup B) = P(A) + P(B) - P(A \cap B)$

- Conditional probability

$P(B|A) = P(A \cap B) / P(A)$. Given A.

(Why ? Multiplicative ! $\Rightarrow \underbrace{P(A)}_{\text{A already happened}} \cdot P(B|A) = \underbrace{P(A \cap B)}_{\text{Then, both A, B happens.}}$)

- Independence.

$P(B|A) = P(B)$: doesn't care A happen.

$\Rightarrow P(A) \cdot P(B) = P(A \cap B)$.

• Random Variables.

• Discrete RV

Event : $\{X = x\}$

$\langle X \rangle = \sum_x x \, P(X = x)$

$Var(X) = \langle (X - \langle X \rangle)^2 \rangle = \langle X^2 + \langle X \rangle^2 - 2 \langle X \rangle X \rangle$

$= \langle X^2 \rangle + \langle X \rangle^2 - 2 \langle X \rangle^2$

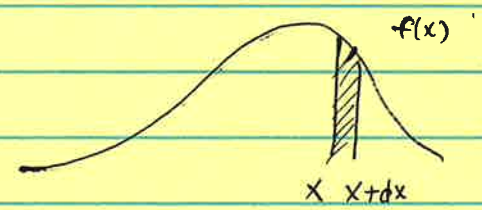
$= \langle X^2 \rangle - \langle X \rangle^2$

$\sigma(X) = \{Var(X)\}^{1/2}$

$\langle X^k \rangle = k^{th}$ moment.

$\langle g(X) \rangle =$ average.

• Continuous RV



$f(x) \cdot dx = P\{x \le X \le x + dx\}$.

$E\{X\} = \int_\Omega x f(x) \, dx$.

$E\{(X - E\{X\})^2\} = Var\{X\}$.

$= \int_\Omega x^2 f(x) \, dx - \left(\int x f(x) dx \right)^2$.

4. • Q) Prove $\langle XY \rangle = \langle X \rangle \langle Y \rangle$ if X, Y are independent

9:45–9:50

A) $\langle XY \rangle = \iint y x \cdot f(x) \cdot f(y) \cdot dx \, dy = \int dy \, y \left(\int dx \cdot x f(x) \right) f(y) = \langle X \rangle \cdot \langle Y \rangle$ #

$\sum x \, P(X = x) \cdot y \, P(Y = y) = \sum xy \, P(X = x, Y = y)$ HW 2-c

• Multi-variate prob. dist.

- $\langle aX + bY \rangle = a\langle X \rangle + b\langle Y \rangle$.
- $\mathrm{cov}(X,Y) = \langle \underbrace{(X - \langle X \rangle)}_{\text{mean}=0,\ \mathrm{Var}(X)} \underbrace{(Y - \langle Y \rangle)}_{\text{mean}=0\ \ \mathrm{Var}(Y).} \rangle \rightsquigarrow \langle \uparrow\uparrow\ ,\ \uparrow\downarrow\ ,\ \downarrow\downarrow \rangle$

$$= \langle XY \rangle - \langle X \rangle\langle Y \rangle \cdot 2 + \langle X \rangle\langle Y \rangle = \langle XY \rangle - \langle X \rangle\langle Y \rangle.$$

- correlation : $\rho(X,Y) = \mathrm{cov}(X,Y) / \sigma_X \sigma_Y$.

Q) $X_1 \sim X_N$ where $X_i \sim N(\mu, \sigma^2)$, i.i.d.

Define $\bar{X} = \frac{1}{N}\sum_{i=1}^{N} X_i$, $\langle \bar{X} \rangle = \mu$, $\mathrm{Var}(\bar{X}) = \sigma^2/N$, $\sigma(\bar{X}) = \sigma/\sqrt{n}$

pf) $\mathrm{Var}(\bar{X}) = \langle (\bar{X} - \langle \bar{X} \rangle)^2 \rangle = \langle \bar{X}^2 \rangle - \langle \bar{X} \rangle^2$

$$= \frac{1}{N^2} \cdot \langle \sim \rangle - \mu^2 = \frac{1}{N^2}\langle X_1^2 + X_2^2 + \cdots + X_N^2 + 2X_1X_2 + \cdots + 2X_{N-1}X_N \rangle - \mu^2$$

$$= \cancel{\frac{1}{N^2}\langle X_1 \cdot \bar{X} N + X_2 \cdot \bar{X} \cdot N + \cdots + X_N \cdot X \cdot N \rangle - \mu^2} \qquad \frac{2}{N^2}\mu^2 \cdot \frac{N \cdot (N-1)}{2}$$

$$= \cancel{\frac{1}{N}\sigma\bar{X}} = \frac{1}{N^2}\sum_i \langle X_i^2 \rangle + \underbrace{\frac{2}{N^2} \cdot \sum_{i \neq j} \langle X_i X_j \rangle}_{\neq 0} - \mu^2$$

$$= \frac{1}{N^2} \cdot \sum_i \{ \mathrm{Var}(X_i) + \mu^2 \} + 0 - \mu^2 = \frac{1}{N^2} \cdot N \cdot \mathrm{Var}(X_i) = \sigma^2/N . \ \#.$$

5 • Central limit Theorem → central limit theorem.

9:10–9:55

6 • Fun : stirling's formula.

9:55–10:00

$$N! = \sqrt{2\pi N} \cdot (N/e)^N \rightarrow \underline{\ln N!} = N \ln N - N + \cdots$$

discrete — continuous — Entropy.

If time permits.

Gaussian distribution

$$\left(\int_{-\infty}^{+\infty} e^{-x^2} dx\right)^2 = \int_{-\infty}^{+\infty} e^{-x^2} dx \cdot \int_{-\infty}^{+\infty} e^{-y^2} dy = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} e^{-(x^2+y^2)} dx\,dy$$

$x = r\cos\theta, \quad y = r\sin\theta.$

~~dxdy~~ $dx\,dy = r\,dr\,d\theta$

$$= \int_0^{2\pi}\int_0^{\infty} e^{-r^2} \cdot r\,dr\,d\theta = 2\pi \cdot \frac{1}{2} = \pi.$$

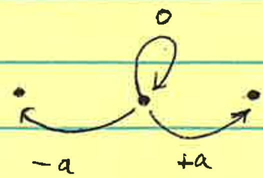
$$\Rightarrow \int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi}.$$

$$\therefore \quad f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\left(\frac{x-\mu}{\sigma}\right)^2\right).$$

Myung Chul Kim.

01/10/2025

Stationary Random Walk.



$$l_i = \begin{cases} +a & \text{prob}: p \\ 0 & \text{prob}: 1-2p \\ -a & \text{prob}: p \end{cases} \qquad (p < 1/2) \quad \text{——} (*)$$

Then, $\langle l_i \rangle = a\cancel{p} + 0 \cdot (1-2p) + \cancel{(-a)} \cdot p = 0$ —— ①

Also, $\langle l_i^2 \rangle = a^2 \cdot p + 0^2 \cdot (1-2p) + (-a)^2 p = 2a^2 p$. —— ②.

we know that $\langle l_i l_j \rangle = \langle l_i \rangle \cdot \langle l_j \rangle = 0$ if $i \neq j$ $\because$ l_i, l_j independent.

From the previous work,

$$\langle |X(n\tau)|^2 \rangle = \left\langle \left(\sum_i l_i \right) \right\rangle^2 = \sum_i \langle l_i^2 \rangle + \cancel{\sum_{i \neq j} \langle l_i l_j \rangle} \to 0.$$
$$= n \cdot (2a^2 p)$$

Recall that $\langle |X(t)|^2 \rangle = 2D_s \cdot t \cdot d$. ($d$: dimension $= 1$.)

$$\Rightarrow \cancel{n} \cdot (\cancel{2} a^2 p) = \cancel{2} \cdot D_s \cdot \cancel{n} \tau \cdot 1$$

$$\Rightarrow D_s = a^2 p / \tau$$

Note that non-stationary case yields $D = \dfrac{a^2}{2\tau}$. and $D_s = \dfrac{a^2}{2\tau}(2p)$.

$$\Rightarrow D_s / D = 2p < 1 \quad (\because *) \quad \therefore D_s < D$$

Q) What is $(2p)$?

Hint : Recall $D = \mu k_B T$ or $D = k_B T / \xi$

ME346A – Introduction to Statistical Mechanics – Wei Cai – Stanford University – Winter 2025

Problem Session 1

January 10, 2025

Proof of Central Limit Theorem (CLT)

Let $X_1, X_2, \ldots, X_N$ be a random sample from an arbitrary distribution with mean μ and variance σ^2. We shall assume that N is sufficiently large. Define,

$$\bar{X} := \frac{1}{N}\sum_{i=1}^{N} X_i,$$

where the expectation and the variance of $\bar{X}$ can be calculated as,

$$\langle \bar{X} \rangle = \frac{1}{N}\sum_{i=1}^{N}\langle X_i \rangle = \mu, \quad \mathrm{Var}(\bar{X}) = \left\langle \left(\bar{X} - \langle \bar{X} \rangle\right)^2 \right\rangle = \langle \bar{X}^2 \rangle - \langle \bar{X} \rangle^2 = \langle \bar{X}^2 \rangle - \mu^2,$$

Recall that $\langle \bar{X}^2 \rangle$ reads,

$$\langle \bar{X}^2 \rangle = \left\langle \left(\frac{1}{N}\sum_{i=1}^{N} X_i\right)\left(\frac{1}{N}\sum_{i=1}^{N} X_i\right) \right\rangle = \frac{1}{N^2}\left(\sum_{i=1}^{N}\langle X_i^2 \rangle + 2\sum_{i\neq j}\langle X_i X_j \rangle\right),$$

and because X_i are independent samples, $\langle X_i X_j \rangle = \langle X_i \rangle \langle X_j \rangle = \mu^2$. Also note that $\langle X_i^2 \rangle = \mathrm{Var}(X_i) + \langle X_i \rangle^2 = \sigma^2 + \mu^2$ so that,

$$\langle \bar{X}^2 \rangle = \frac{1}{N^2}\left(N\left(\sigma^2 + \mu^2\right) + 2\binom{N}{2}\mu^2\right) = \frac{\sigma^2 + \mu^2}{N} + \frac{N-1}{N}\mu^2 = \frac{\sigma^2}{N} + \mu^2,$$

so that the expectation and the variance of $\bar{X}$ is,

$$\boxed{\langle \bar{X} \rangle = \mu, \quad \mathrm{Var}(\bar{X}) = \frac{\sigma^2}{N}.}$$

Semi-Stationary Random Walk

Let us define a semi-stationary random walk, which is described as a random walker in 1-dimensional space. At each time step, the random walker can move either $+a$ or $-a$ with probability p and also can stay at its state with probability $1-2p$. We call this random walk as semi-stationary because the random walker can stay where it is.

Define a step that the random walker takes at i^{th} time step to be l_i. Then, the expectation of l_i and l_i^2 can be calculated as,

$$\langle l_i \rangle = (+a)p + (0)(1-2p) + (-a)p = 0, \quad \langle l_i^2 \rangle = (a^2)p + 0^2(1-2p) + (a^2)p = 2a^2p,$$

which can be used to calculate $\langle |X(n\tau)|^2 \rangle$ as,

$$\langle |X(n\tau)|^2 \rangle = \left\langle \left(\sum_i l_i \right)^2 \right\rangle = \sum_i \langle l_i^2 \rangle = n(2a^2p),$$

assuming that l_i and l_j are independent when $i \neq j$. Recall that $\langle |X(n\tau)|^2 \rangle = 2D_s n\tau$,

$$2D_s n\tau = n(2a^2p), \quad D_s = 2pD$$

where $D = a^2/(2\tau)$ and D_s is a diffusion coefficient for the semi-stationary random walk. Hence, we have derived that the probability of moving in the semi-stationary random walk drives the mobility of the diffusion. In other words, the action of staying at its state works as a friction which slows down the diffusion.

Problem Session 2 01/17/2025.

Lagrangian. 09:30 - 09:40

$F_i = m \cdot \ddot{q}_i \Leftrightarrow dp_i/dt = F_i \Leftrightarrow \ddot{q}_i = -\frac{1}{m} \cdot \partial U/\partial q_i$ (Newton, 1687)

Define,

$\mathcal{L}(\{q_i\}, \{\dot{q}_i\}) = K - U = \sum_i \left(\frac{1}{2} m \dot{q}_i^2 - U(q_i)\right)$ where,

$\frac{d}{dt}\left(\partial L/\partial \dot{q}_i\right) - \left(\partial L/\partial q_i\right) = 0$ for $\forall t$ (Lagrange, 1760)

pf) $\partial L/\partial \dot{q}_i = m \cdot \dot{q}_i \equiv p_i$

$\partial L/\partial q_i = -\partial U/\partial q_i$

$\Rightarrow \frac{d}{dt} p_i = -\partial U/\partial q_i = F_i$

Using derivatives,

$dL = \sum_i \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i$

$\Rightarrow \frac{dL}{dt} = \sum_i \underbrace{\frac{\partial L}{\partial q_i} dq_i/dt}_{= ①} + \underbrace{\frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i/dt}_{= \frac{\partial L}{\partial \dot{q}_i} \frac{d}{dt}(\dot{q}_i)}$

$① = \frac{\partial L}{\partial q_i} \frac{dq_i}{dt} = \left(\partial L/\partial q_i\right) \cdot \left(\partial \dot{q}_i/\partial q_i\right) \cdot \underbrace{\frac{dq_i}{dt}}_{= \dot{q}_i} = \underbrace{\left(\partial \dot{q}_i/\partial q_i\right)}_{= d/dt}\left(\partial L/\partial \dot{q}_i\right) \cdot \dot{q}_i$

$= \frac{d}{dt}\left(\partial L/\partial \dot{q}_i\right) \dot{q}_i$

$\Rightarrow dL/dt = \sum_i \frac{d}{dt}\left(\partial L/\partial \dot{q}_i\right) \dot{q}_i + \partial L/\partial \dot{q}_i \frac{d}{dt}(\dot{q}_i) = \sum_i \frac{d}{dt} \cdot \left(\partial L/\partial \dot{q}_i\right) \dot{q}_i$

$\therefore \frac{d}{dt}\left[L - \sum_i \frac{\partial L}{\partial \dot{q}_i} \dot{q}_i\right] = 0$

Hamiltonian 09:40 - 09:50

Define $\underbrace{H = -L + \sum_i (\partial L/\partial \dot{q}_i)\dot{q}_i}_{\text{Legendre's Transform (1787)}} \Rightarrow \frac{d}{dt}(H) = 0 \Rightarrow H$ is conserved.

$\langle L \to H \rangle$

Note : $H = -L + \sum_i (\partial L/\partial \dot{q}_i)\dot{q}_i$ and $\partial L/\partial \dot{q}_i = m \cdot \dot{q}_i \equiv p_i$

$\Rightarrow H = -L + \sum_i p_i \dot{q}_i$

(*) $\boxed{dH = \sum_i \dot{q}_i\, dp_i - \dot{p}_i\, dq_i}$

Also, $\partial L/\partial q_i = \frac{d}{dt}(\partial L/\partial \dot{q}_i) = \dot{p}_i \rightsquigarrow$ Force?!

$\therefore \partial L/\partial \dot{q}_i \equiv p_i$
$\partial L/\partial q_i \equiv \dot{p}_i$

$$dH = \sum_i \cancel{p_i\, d\dot{q}_i} + \dot{q}_i\, dp_i - \underbrace{\frac{\partial L}{\partial q_i}}_{=\dot{p}_i} dq_i - \cancel{\underbrace{\frac{\partial L}{\partial \dot{q}_i}}_{=p_i} d\dot{q}_i}$$

$\boxed{\text{Key point : Legendre Transform eliminates the dependence of the function } L \text{ respect to the variable } \dot{q}_i}$

Example)

① $H(p, x) = \frac{p^2}{2m} + U(x)$: Function of p, x.

I want to replace "p" with something else!

$\Rightarrow L = H - \left(\frac{\partial H}{\partial p}\right)_x \cdot p = H - v \cdot p \quad \left(\because \frac{\partial}{\partial p}\left(\frac{p^2}{2m}\right) = p/m = v\right)$

$\Rightarrow L = H - v \cdot p$: ~~Constant~~ For x and v

check : ① $dH = \left(\frac{\partial H}{\partial p}\right)_x dp + \left(\frac{\partial H}{\partial x}\right)_p dx = (v)_x\, dp + (U'(x))_p\, dx$ $\boxed{\text{Function of } (p, x)}$

② $dL = dH - v\,dp - p\,dv = \cancel{v\,dp} + U'(x)\,dx - \cancel{v\,dp} - p\,dv$

$= U'(x)\,dx - p\,dv$ $\boxed{\text{Function of } (v, x)}$

Note : From (*)

$dH = \sum_i -\dot{p}_i\, dq_i + \dot{q}_i\, dp_i$

$dH = \sum_i \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i$

< Eq. motion Hamilt. >

$\dot{p}_i = -\partial H/\partial q_i$

$\dot{q}_i = \partial H/\partial p_i$

- Example on Thermodynamics.

$E = TS - pV + \mu N$ and $dE = TdS - pdV + \mu dN$

$\searrow E(S, V, N)$

Free Energy.

① $E - \underbrace{\left(\partial E/\partial S\right)_{V,N}}_{T} S \equiv A$ (Helmholtz)

$dA = dE - TdS - SdT = \cancel{TdS} - pdV + \mu dN - \cancel{TdS} - SdT$ $\boxed{N, V, T}$

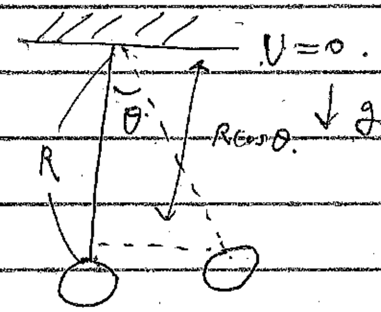
② $E - TS - \underbrace{\left(\partial E/\partial V\right)_{S,N}}_{= -p} V \equiv G$ (Gibbs)

$dG = \cancel{TdS} - \cancel{pdV} + \mu dN + \cancel{pdV} - \cancel{TdS} - SdT + Vdp$ $\boxed{N, P, T}$

- Example on pendulum. **09:40 - 09:50**

① $K = \frac{1}{2} m \cdot v^2$

$= \frac{1}{2} m (R\dot{\theta})^2 = \frac{1}{2} mR^2 (\dot{\theta})^2$



$U = - mgR \cdot \cos\theta$.

Formulate Lagrangian as,

$\Rightarrow L = K - U = \frac{1}{2} mR^2 (\dot{\theta})^2 + mgR\cos\theta$.

$\searrow$ function of θ, $\dot{\theta}$

② Equation of motion.

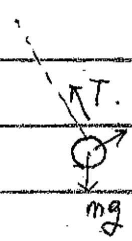
1) Lagrangian

$\frac{d}{dt}\left(\partial L/\partial \dot{\theta}\right) - \partial L/\partial\theta = 0$

$\Rightarrow \frac{d}{dt}\left(mR^2 \cdot \dot{\theta}\right) - \left(-mgR\sin\theta\right) = 0$

$\Rightarrow \ddot{\theta} = -g/R \cdot \sin\theta$

2) Newtonian



$T = mg \cdot \cos\theta$

$m\ddot{\theta}R - mg\sin\theta = m \cdot R\ddot{\theta}$

$\Rightarrow \ddot{\theta} = - g/R \cdot \sin\theta$.

③ To Hamiltonian, (by Legendre Transform).

$L(\theta, \dot\theta)$ → we want to eliminate $\dot\theta$

$H^{+} = -L + \left(\partial L / \partial\dot\theta\right)\dot\theta$ where $p_\theta = \partial L / \partial \dot\theta = mR^2\dot\theta$

$= \frac{-1}{2} mR^2(\dot\theta)^2 \cancel{+} mgR\cos\theta + mR^2 \cdot \dot\theta \cdot \dot\theta$

$= -mgR\cos\theta + p_\theta^2/(2mR^2)$ (sign flip okay).

$H^{+} = p_\theta^2/(2mR^2) - mgR\cos\theta$.

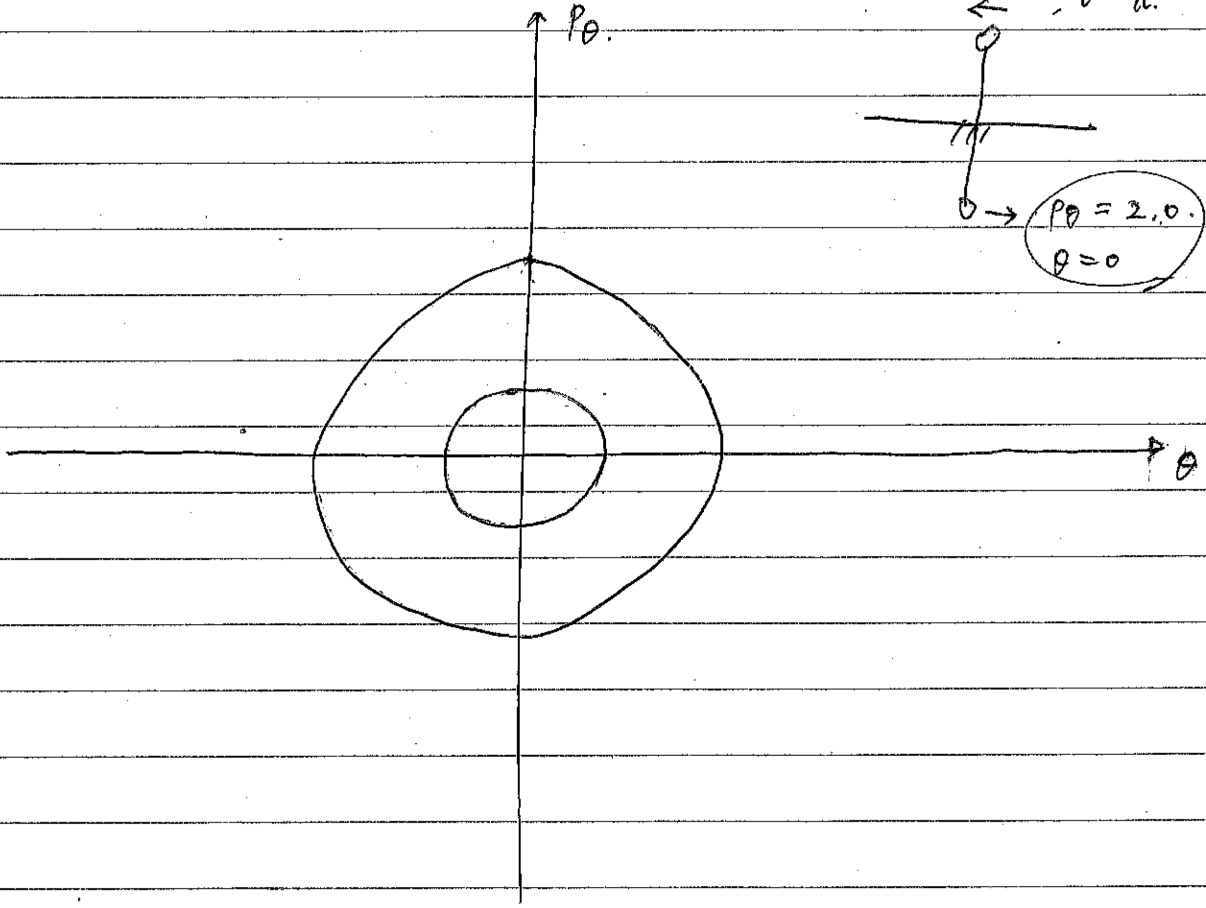
Recall eq. mot. Hamilt. **09:50 - 10:00**

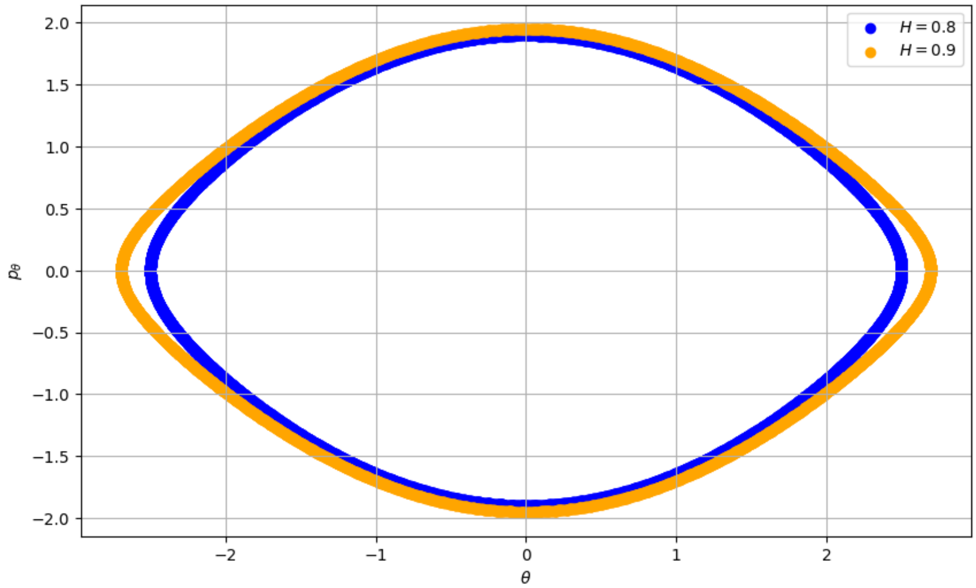
$\dot p_i = -\partial H/\partial q_i = -(-mgR.(-\sin\theta)) = -mgR\sin\theta$.

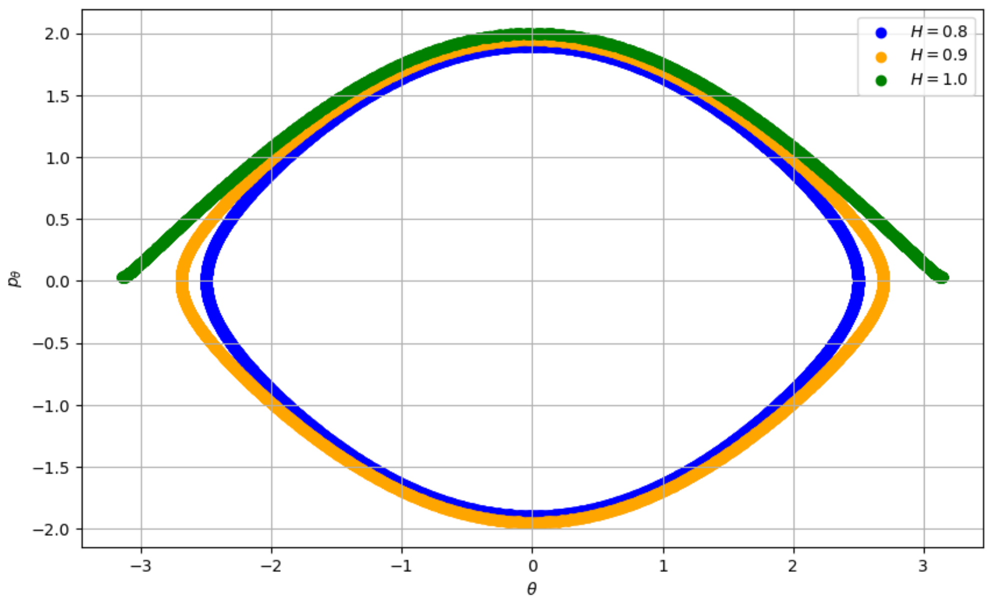
$\dot q_i = +\partial H/\partial p_i = p_\theta/(mR^2)$

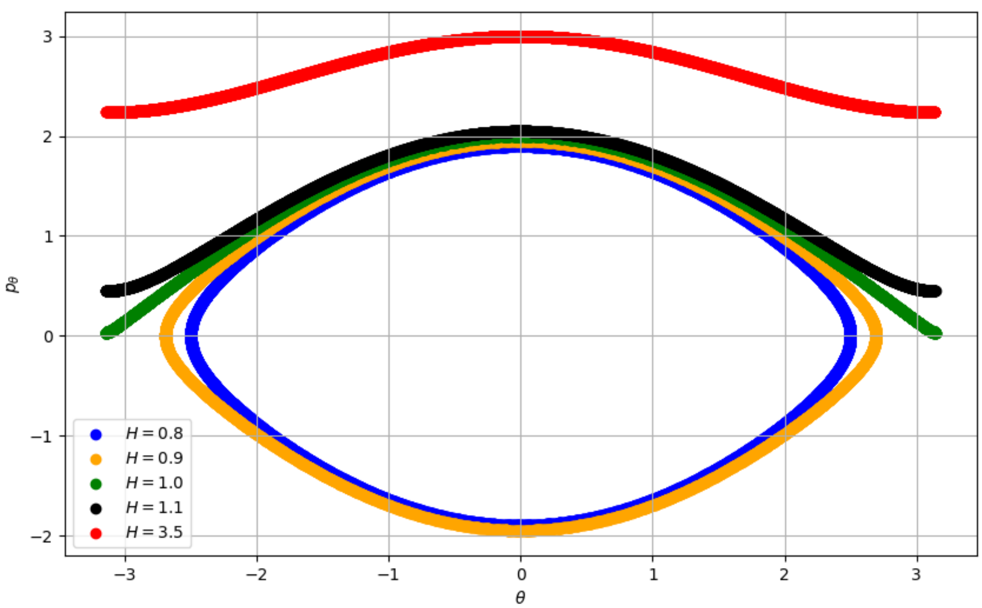
$H = 1$

$V=0$, $\theta = \pi$.




$H = 0.8$
$H = 0.9$
p_θ
θ


$H = 0.8$
$H = 0.9$
$H = 1.0$
p_θ
θ


$H = 0.8$
$H = 0.9$
$H = 1.0$
$H = 1.1$
$H = 3.5$
p_θ
θ

ME 346A Problem Session (01/31/2025)

- Properties of Ideal Gas. (p. 24 – 27 of notes), Ch. 6.

$$S = k_B \cdot N \cdot \left[\frac{5}{2} + \log\left(\frac{V}{N} \cdot \left(\frac{4\pi m E}{3 N h^2} \right)^{3/2} \right) \right]$$

(Refer p.10 Ch7 for derivation with hypersphere assumption)

09:30-09:40

(a) $E(S, V, N) = ?$, $T = ?$, $p = ?$ $\mu = ?$

Does $pV = Nk_BT$ hold?

$$E(S,V,N) = \frac{3Nh^2}{4\pi m} \left(\frac{N}{V} \right)^{2/3} \exp\left[\frac{2S}{3Nk_B} - \frac{5}{3} \right]$$

$V^{-2/3}$

① $T = \left(\partial E / \partial S \right)_{V,N} = \frac{2}{3Nk_B} \cdot E(S,V,N) \Rightarrow E = \frac{3}{2} N k_B T.$

② $p = -\left(\partial E / \partial V \right)_{S,N} = -\left(-2/3 \cdot V^{-5/3} \cdot ① \right) = \frac{2}{3} \frac{1}{V} E$

$= Nk_BT / V \Rightarrow pV = Nk_BT.$

③ $\mu = \left(\partial E / \partial N \right)_{S,V} = E/N \cdot \left(5/3 - 2S/(3Nk_B) \right)$

09:40-09:50

(b) $A = E - TS = \frac{3}{2} N k_B T - T N k_B \cdot \left[\log\left(\frac{V}{N} \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} \right) + 5/2 \right]$

(c) $G = E - TS + pV = A + pV$

$= -Nk_BT \left[\log\left(\frac{k_BT}{p} \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} \right) \right]$

From ③ of (a),

$\mu N = E \left(5/3 - 2S/(3Nk_B) \right) = \frac{5}{2} Nk_BT - TS$

$= G \Rightarrow G = \mu N.$

09:50-10:00

(d) $C_V = \left(đQ/dT\right)_{V,N} = T\cdot\left(\frac{\partial S}{\partial T}\right)_{V,N} = -T\cdot\left(\partial^2 A/\partial T^2\right)_{V,N}.$

since $S = -\left(\partial A/\partial T\right)_{N,V}$

$\because A = E - T\cdot S$

$$\Rightarrow \boxed{C_V = T\left(\frac{\partial S}{\partial T}\right) = \frac{3}{2} N k_B.}$$

$C_p = \left(đQ/dT\right)_{p,N} = T\left(\partial S/\partial T\right)_{p,N} = -T\left(\partial^2 G/\partial T^2\right)_{p,N}.$

since $S = -\left(\partial G/\partial T\right)_{p,N}$

$\because G = E - TS + pV$

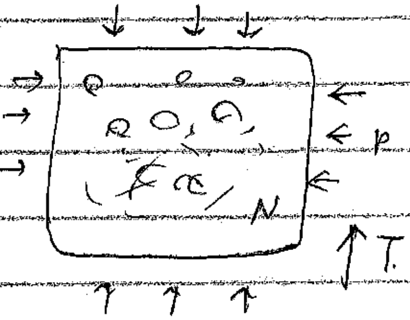
$$\Rightarrow \boxed{C_p = \frac{5}{2} N k_B.}$$

$$\Rightarrow C_p - C_V = N k_B.$$

10:00-10:10

(e) At constant pressure, and fixed N, we want to know

$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{p,N}$



From $pV = Nk_BT$, $V = Nk_BT/p$.

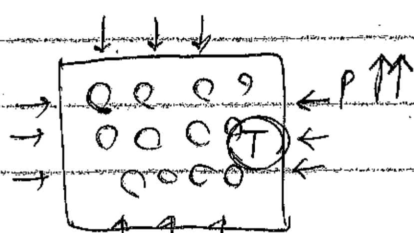
$\Rightarrow \alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{N,p} = \frac{p}{Nk_BT}\cdot\frac{Nk_B}{p} = 1/T$

$$\Rightarrow \boxed{\alpha = 1/T}$$

At constant temperature, and fixed N, we want to know.

$\beta = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_{T,N}$

$\beta = +\frac{1}{V}\cdot\left(\frac{Nk_BT}{p^2}\right) = 1/p.$



$$\Rightarrow \boxed{\beta = 1/p}$$

$\alpha^2 VT/\beta = \frac{1}{T^2} VTp$

$= Nk_B = C_p - C_V.$

10:10-10:20

Notes on Legendre Transform & Laplace Transform

$$Z(\beta) = \sum_{\nu \mid \cancel{E(\nu) = E}} e^{-\beta E(\nu)} \approx \underbrace{\int dE \cdot \Omega(E) \cdot e^{-\beta E(\nu)}}_{} \quad : \text{Laplace Transform} \quad ①$$

$$① = \int dE \cdot \Omega(E)\, e^{-\beta E(\nu)} = \int d\varepsilon \cdot \exp\Big[\underbrace{-N(\underbrace{\beta\varepsilon - \log w(\varepsilon)}_{= a(\varepsilon)})}_{= A(E)} \Big]$$

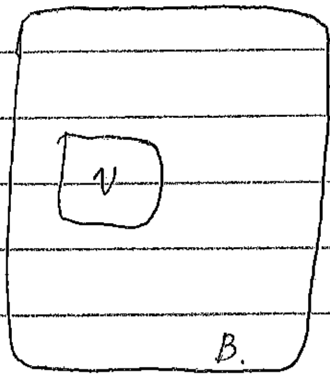
where $A = E - T \cdot S = E - \left(\partial E / \partial S\right)_{N,V} \cdot S$: Legendre Transform ②

① & ② are related.

< Optional >

ME346A Problem Session. (01/31/2025). 01/27/2025.

• Micro-Canonical Ensemble.



$E_T = E(\nu) + E_B.$ → partition function.

$p(\nu, B) = 1 / \Omega(N_T, V_T, E_T)$

$\Rightarrow p(\nu) = \sum_{\{B \mid E(\nu)+E(B)=E(T)\}} p(\nu, B) = \frac{1}{\Omega_T} \cdot \Omega_B.$

$\Rightarrow p(\nu) = \frac{1}{\Omega_T} \cdot \Omega_B(E_T - E(\nu), N_B, V_B)$

$N_T, V_T, E_T \to$ Fixed.

$$\log p(\nu) \propto \log \Omega_B(E_T - E(\nu), N_B, V_B) = \log \Omega_B(E_T) - \left(\frac{\partial \log \Omega_B(N_B, V_B, E_B)}{\partial E_B}\right) \cdot E(\nu) + \cancel{O((E(\nu))^2)} \to 0$$

$$\Rightarrow \log p(\nu) \propto -\underbrace{\left(\partial \log \Omega_B / \partial E_B\right)_{N_B, V_B}}_{(=\beta.)} E(\nu).$$

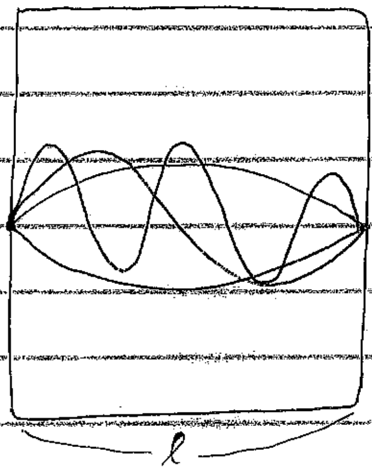
$\Rightarrow p(\nu) \propto e^{-\beta E(\nu)}$; Boltzmann Distribution!

$$Z(\beta) = \sum_{\nu} e^{-\beta E(\nu)} = \sum_{E} \Omega(E) \cdot e^{-\beta E}. \quad \langle \text{Laplace} \rangle$$

$$\Rightarrow \approx \int dE\, \Omega(E)\, e^{-\beta E(\nu)} = \int dE \exp\left(-\beta [E - \beta^{-1} \log \Omega(E)]\right)$$

$$= \int dE \exp\left(-N\beta \cdot (\underbrace{\varepsilon - Ts}_{=a})\right) \quad \langle \text{Legendre} \rangle$$

- Ideal Gas Law.



→ Translational only,

Quantum Mechanics : $\frac{n^2 h^2}{8 m l^2} = \varepsilon_n$ (quantized)

$$z(\beta) = \sum_{n=1}^{\infty} e^{-\beta \varepsilon_n}.$$

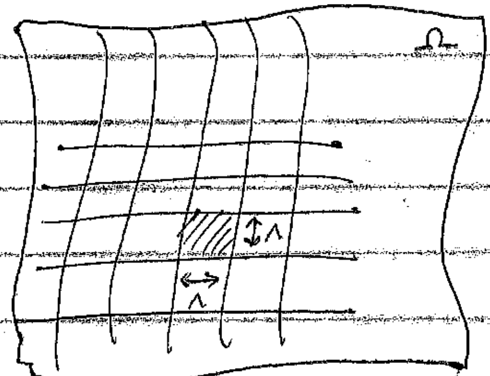
$$z(\beta) \approx \int_0^{\infty} e^{-\beta \varepsilon_n}\, dn = \frac{\sqrt{2\pi m k_B T}}{h} \quad (\beta << 1)$$

— ②

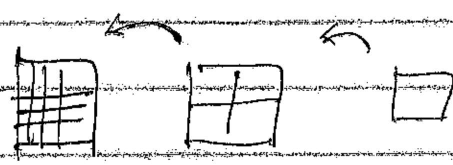
Extend ② to 3D, $\varepsilon_{n,3D} = \frac{h^2}{8m^2}\left[(n_x/l_x)^2 + (n_y/l_y)^2 + (n_z/l_z)^2 \right]$

$$\Rightarrow z(\beta)_{3D} = \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} \cdot l_x l_y l_z = V/\Lambda^3 \quad \left(\Lambda = \left(\sqrt{2\pi m k_B T}/h \right)^{-1} \right)$$

small z



Λ : Thermal De Broglie wavelength.



$$A = -\beta^{-1} \cdot \log Z(\beta), \quad A = E - TS, \quad Z(\beta) = \frac{1}{N!}(z(\beta))^N$$

$$\Rightarrow -p = \partial A/\partial V \Big|_{N,T} = -\beta^{-1} \cdot \partial/\partial V \left(\frac{1}{N!} \log \left(V/\Lambda^3 \right)^N \right) = -\beta^{-1} \cdot \frac{N}{V}$$

$$\boxed{\therefore\ pV = N \cdot k_B T. \iff \beta P = \rho.}$$

- From Quantum Mechanics Partition Function.

$$Z(\beta) = {}^{1}/_{N!} \; z^{N}(\beta) \quad \left(\text{where} \quad z(\beta) = V/\Lambda^{3} \right)$$

$$\langle E \rangle = \frac{\partial}{\partial(-\beta)} \log Z(\beta) = N k_B T^2 \left(\frac{\partial}{\partial T} \log z(\beta) \right)_{N,V}$$

$$= N k_B T^2 . \frac{\frac{3}{2} \cdot \left(\frac{2\pi m k_B T}{h^2} \right)^{1/2} \frac{2\pi m k_B}{h^2}}{\left(\frac{2\pi m k_B T}{h^2} \right)^{3/2}} = \frac{3}{2} N k_B T^2 \frac{1/\Lambda \; 1/\Lambda^{0}}{1/\Lambda^{3}} \frac{1}{T}$$

$$\Rightarrow \boxed{\langle E \rangle = \frac{3}{2} N k_B T.} \qquad \text{as } N \to \infty, \; E = \frac{3}{2} N k_B T \quad (\because \text{var}(E) \downarrow 0)$$

- Some thermo-properties.

$$p = -\left(\partial E / \partial V \right)_{S,N} = N k_B T / V$$

$$\mu = \left(\partial E / \partial N \right)_{S,V} = \frac{3}{2} k_B T .$$

$$\alpha = \frac{1}{V} \left(\partial V / \partial T \right)\Big|_{p} = 1/T , \qquad \gamma = -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_{T,N} = 1/p.$$

$\Rightarrow$ Similar to. Sackur – Tetrode equation.

Problemm Session 02/07/2025.

09:30 → 09:40 Ideal Gas.

$$Z = \frac{1}{N!}\frac{1}{h^{3N}} \cdot \int \prod_{i=1}^{3N} dq_i\, dp_i \exp\left(-\frac{H(\{q_i\},\{p_i\})}{k_B T}\right).$$

$$H = \sum_i \frac{|p_i|^2}{2m} + \cancel{V(\{q_i\})} \to 0.$$

$$\Rightarrow Z = \frac{1}{N!}\frac{1}{h^{3N}} \int \prod_{i=1}^{3N} dq_i\, dp_i \exp\left(-\frac{p^2}{2mk_BT}\right)$$

$$= \frac{1}{N!}\frac{1}{h^{3N}} \cdot V \cdot \left[\int_{-\infty}^{\infty} dp \cdot \exp\left(-\frac{p^2}{2mk_BT}\right)\right]^{3N}$$

$$= \frac{V^N}{N!\,h^{3N}} (2\pi m k_B T)^{3N/2}$$

$$\therefore Z = \frac{V^N}{N!\,h^{3N}} (2\pi m k_B T)^{3N/2} \quad \text{——— ①}$$

$$\therefore A = -k_BT \ln Z = -k_B T \cdot N\left[\ln\left(\frac{V}{N}\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}\right) + 1\right]. \quad \#$$

09:40 → 09:45. Quantumm (if time allows).

$$\varepsilon_n = \frac{n^2 h^2}{8ml^2} \Rightarrow z = \sum_{n=1}^{\infty} e^{-\beta \varepsilon_n} = \frac{\sqrt{2\pi m k_B T}}{h} \quad (\beta \ll 1).$$

In 3D, $z = \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} \cdot l_x l_y l_z = V/\Lambda^3$

With N particles, $z^N \cdot \frac{1}{N!} = \frac{V^N}{N!\,h^{3N}} (2\pi m k_B T)^{3N/2}$ ——— ②

$\therefore$ ② recovers ①,

At high temp limit, classical $\approx$ quantumm.

09 : 45 → 09:55 Molecules. with 3 energy.

$E = 2\varepsilon$ — — — … —

$E = \varepsilon$ — — — … —

$E = 0$ — — — … —

1 2 3 … N

$$\cancel{Z = \sum_{i=1}^{N}} \qquad Z = \sum_{\{n_i\}} e^{-\beta H} \qquad H = \sum_{i=1}^{N} \varepsilon n_i$$

1-1)
$$e^{-\beta H} = \exp\left(-\beta \cdot \varepsilon \cdot \sum_{i=1}^{N} n_i\right) = \exp(-\beta \varepsilon n_1) \cdot \exp(-\beta \varepsilon n_2) \cdots$$
$$= \underline{\prod_{i=1}^{N} e^{-\beta \varepsilon n_i}}$$

1-2)
$$\Rightarrow Z = \sum_{\{n_i\}} \prod_{i=1}^{N} e^{-\beta \varepsilon n_i} = \prod_{i=1}^{N} \left(\sum_{n_i = 0,1,2} e^{-\beta \varepsilon n_i} \right)$$
$$= \underline{\left(1 + e^{-\beta \varepsilon} + e^{-2\beta \varepsilon}\right)^N}$$

2)
$$A = -k_B T \cdot \ln Z = -N k_B T \ln\left(1 + e^{-\beta \varepsilon} + e^{-2\beta \varepsilon}\right)$$
$$S = -\partial A / \partial T = -N k_B \cdot \ln\left(1 + e^{-\beta \varepsilon} + e^{-2\beta \varepsilon}\right) - N k_B T \cdot \frac{\left(-\varepsilon \cdot e^{-\beta \varepsilon} + (-2\varepsilon e^{-2\beta \varepsilon}\right)}{1 + e^{-\beta \varepsilon} + e^{-2\beta \varepsilon}} \left(-\frac{1}{k_B T^2}\right)$$

$$\Rightarrow S = N k_B \cdot \ln\left(1 + e^{-\beta \varepsilon} + e^{-2\beta \varepsilon}\right) + \underbrace{N k_B T \cdot \frac{1}{k_B T^2}}_{= N/T} \frac{\varepsilon e^{-\beta \varepsilon} + 2\varepsilon e^{-2\beta \varepsilon}}{1 + e^{-\beta \varepsilon} + e^{-2\beta \varepsilon}}$$

$$E = A + TS = \underline{\frac{N\left(\varepsilon \cdot e^{-\beta \varepsilon} + 2\varepsilon e^{-2\beta \varepsilon}\right)}{1 + e^{-\beta \varepsilon} + e^{-2\beta \varepsilon}}}$$

≈ Expectation. !

09:55 → 10:03) $\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = \frac{\partial \cdot \log(Z)}{\partial(-\beta)} = \frac{\partial}{\partial(-\beta)} \cdot N \cdot \log\left(1 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}\right).$

$$= \underbrace{\frac{\varepsilon e^{-\beta\varepsilon} + 2\varepsilon e^{-2\beta\varepsilon}}{1 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}}}_{\sim \text{Expectation.}} \cdot N \cdot \qquad = N \cdot \varepsilon \left(\frac{e^{-\beta\varepsilon} + 2e^{-2\beta\varepsilon}}{1 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}} \right)$$

10:00 → 10:05 4) Heat capacity,

$$C_V = \left(\partial E / \partial T \right)_N$$

$$= \frac{\partial \beta}{\partial T} \cdot \frac{\partial E}{\partial \beta} = -\frac{1}{k_B T^2} \frac{\partial E}{\partial \beta} = \frac{1}{k_B T^2} \cdot \partial E / \partial(-\beta).$$

$$= \frac{1}{k_B T^2} \cdot N \cdot \varepsilon \cdot \left[\frac{\left(\varepsilon e^{-\beta\varepsilon} + 4\varepsilon e^{-2\beta\varepsilon}\right)\left(1 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}\right) - \left(e^{-\beta\varepsilon} + 2e^{-2\beta\varepsilon}\right)(\varepsilon)\left(e^{-\beta\varepsilon} + 2e^{-2\beta\varepsilon}\right)}{\left(1 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}\right)^2} \right]$$

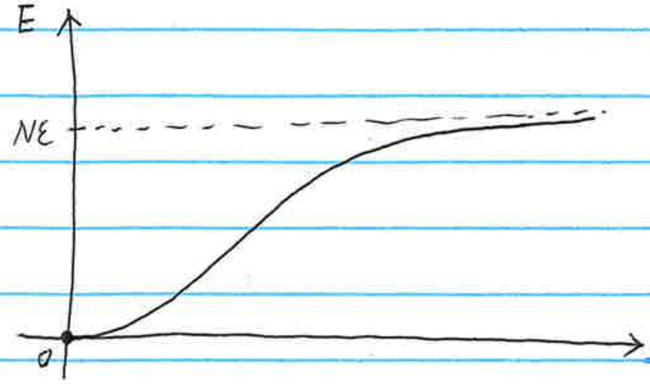
$$= \frac{1}{k_B T^2} \cdot N(1). \left[\underbrace{\frac{\varepsilon^2 e^{-\beta\varepsilon} + 4\varepsilon^2 e^{-2\beta\varepsilon}}{1 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}}}_{=\ \langle \varepsilon^2 \rangle} - \underbrace{\left(\frac{\varepsilon e^{-\beta\varepsilon} + 2\varepsilon e^{-2\beta\varepsilon}}{1 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}} \right)^2}_{\langle \varepsilon \rangle^2} \right]$$

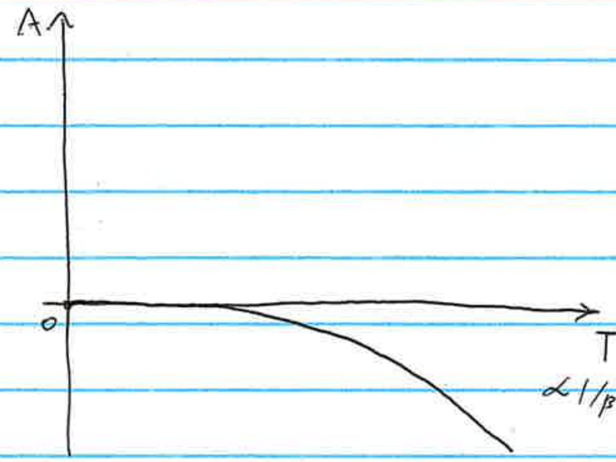
$$= \langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2 = \underline{\mathrm{Var}(\varepsilon)} \,/\!/$$

$$A = -Nk_BT\cdot\ln\left(1+e^{-\beta\varepsilon}+e^{-2\beta\varepsilon}\right)$$

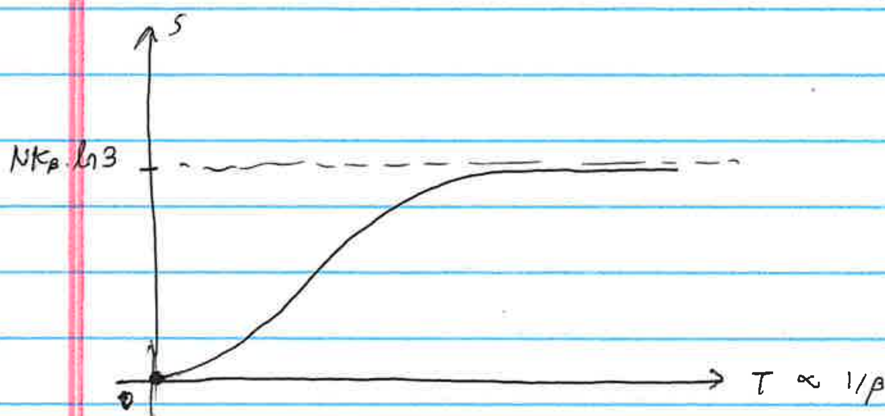
10:05 → 10:15 5)

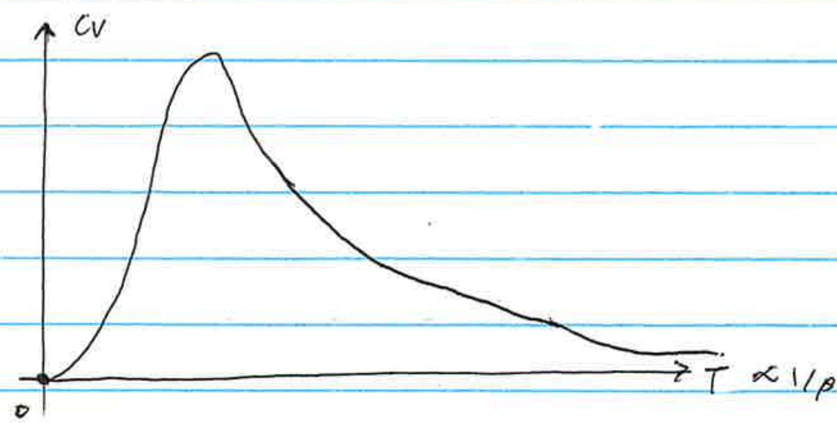
$$E = N\left(\frac{\varepsilon\cdot e^{-\beta\varepsilon}+2\varepsilon e^{-2\beta\varepsilon}}{1+e^{-\beta\varepsilon}+e^{-2\beta\varepsilon}}\right).$$



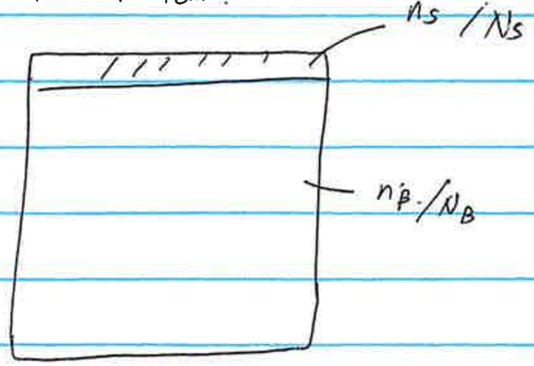


$$S = Nk_B\cdot\ln\left(1+e^{-\beta\varepsilon}+e^{-2\beta\varepsilon}\right)+\underbrace{\frac{N\cdot\beta}{k_B\cdot\beta}}_{=N/T}\cdot\frac{\varepsilon e^{-\beta\varepsilon}+2\varepsilon e^{-2\beta\varepsilon}}{1+e^{-\beta\varepsilon}+e^{-2\beta\varepsilon}}$$





10:15 → 10:30 . Example Problem.



$n = n_s + n_B$.

(a) $E_s = -n_s \cdot \varepsilon$

$S_s = k_B \cdot \ln\left(\frac{N_s!}{n_s!\,(N_s-n_s)!}\right)$

$A_s = E_s - T \cdot S_s = -n_s \cdot \varepsilon - T \cdot k_B \cdot \ln\left[\binom{N_s}{n_s}\right]$

(b) $E_B = \cancel{-n_B \varepsilon}\ 0$

$S_B = k_B \cdot \ln\left(\frac{N_B!}{n_B!\,(N_B-n_B)!}\right)$

$A_B = E_B - T \cdot S_B = \underbrace{\cancel{-n_B \varepsilon}}_{0} - T \cdot k_B \cdot \ln\left[\binom{N_B}{n_B}\right]$

(c) Using sterling's formula,

$A_s \approx -n_s \cdot \varepsilon - k_B T \cdot \left[N_s \cdot \ln N_s - n_s \ln n_s - (N_s - n_s)\ln(N_s - n_s)\right]$

$A_B \approx 0 - k_B T \left[N_B \ln N_B - n_B \ln n_B - (N_B - n_B)\ln(N_B - n_B)\right]$

$\partial A / \partial n_s = -\varepsilon + k_B T \left[\ln n_s + 1 - \ln(N_s - n_s) - 1 \right]$

$A = A_s + A_B$

$- k_B T \left[\ln n_B + 1 - \ln(N_B - n_B) - 1 \right]$ $\quad (\because\ n - n_s = n_B)$

$= -\varepsilon - k_B T \cdot \ln\left[\frac{(N_s - n_s)(n - n_s)}{n_s (N_B - n_B)}\right]$

Using, $N_s, N_B \gg n_s, n_B \Rightarrow \partial A / \partial n_s \cong -\varepsilon - k_B T \cdot \ln\left[\frac{(n - n_s) N_s}{n_s \cdot N_B}\right] = 0$

(d) In (c), reads,

$$n_s = \frac{N_s \cdot n}{N_B \cdot \exp(-\beta \varepsilon) + N_s} \quad \text{—— } (*)$$

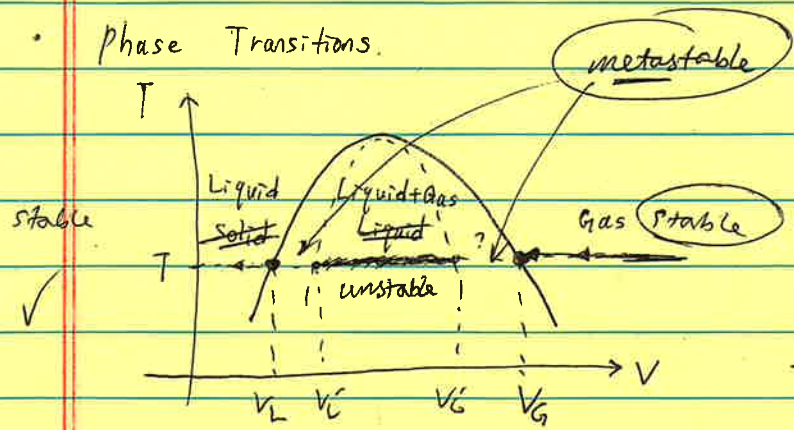
Also, $\partial A_s / \partial n_s = -\varepsilon - k_B T \cdot \ln\left(\frac{N_s - n_s}{n_s}\right) = \mu_s$

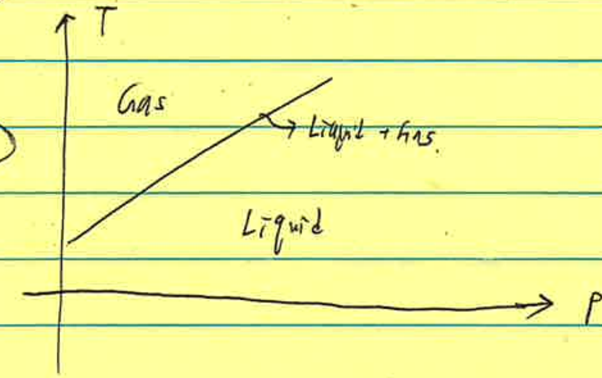
$$\partial A_B / \partial n_B = k_B T \ln\left(\frac{N_B - n_B}{n_B}\right) = \mu_B.$$

$\mu_s = \mu_B$ recovers $(*)$ from Free energy minimization.

Free Energy Minimization $\equiv$ Chemical Potential equilization. #.

- Phase Transitions.



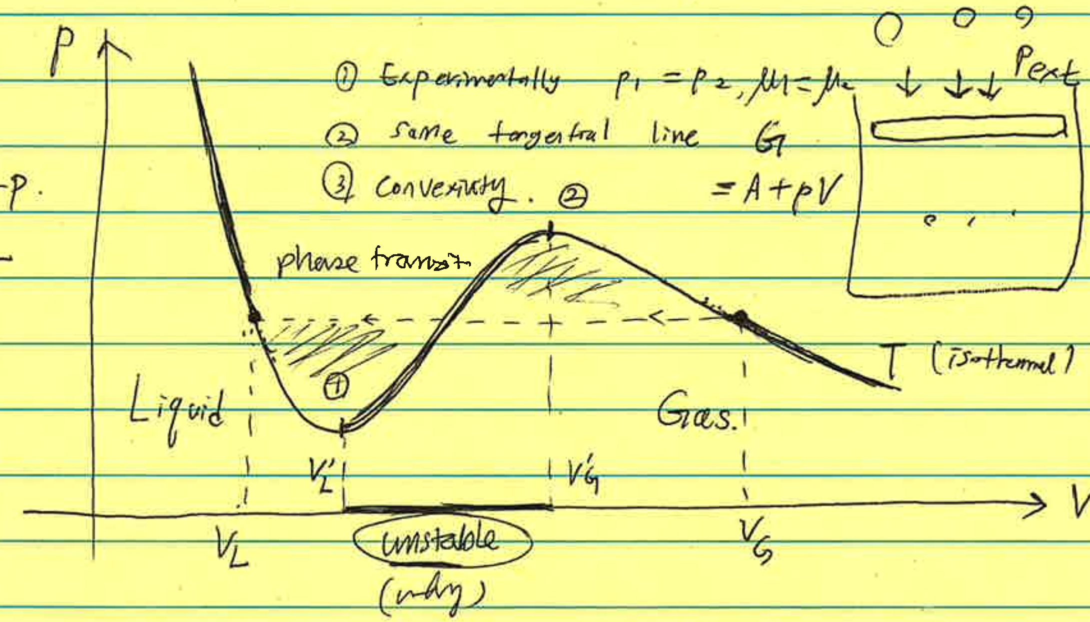


$$\left.\frac{\partial A}{\partial V}\right|_T = -p.$$

① Experimentally $p_1 = p_2$, $\mu_1 = \mu_2$

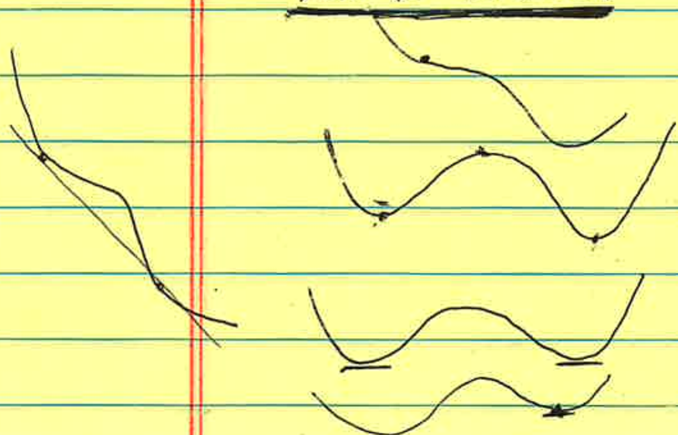
② same tangential line $G = A + pV$

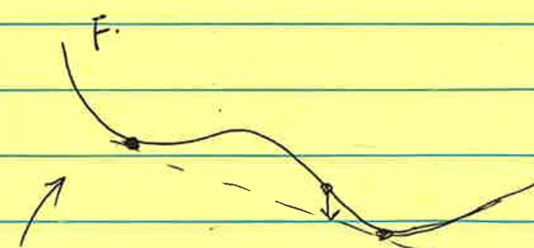
③ Convexity.



In region ① ②, in a cylinder, decreasing P_{ext} slightly will introduce increase in volume, Such volume increase (according to graph ①②), will increase the pressure. Then, again, volume increases. Reapeats → Unstable.

⇒ Maxwell's construction $\quad \left.\partial p/\partial V\right|_T < 0 \quad$ (neccessary for stability)



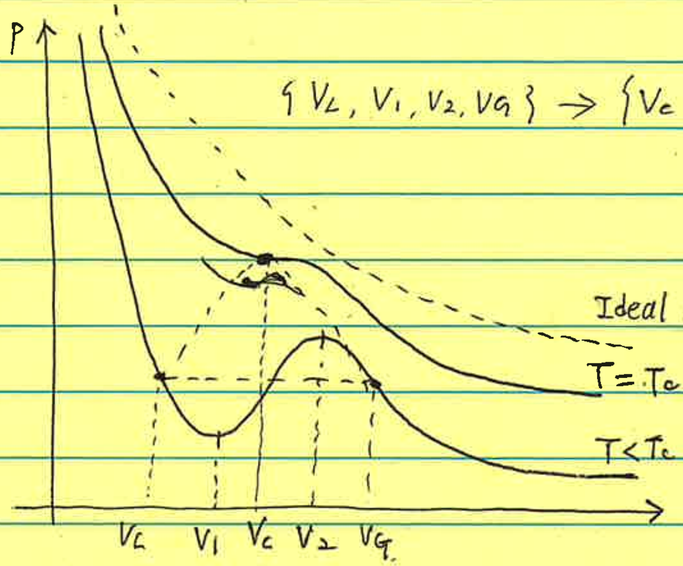


$$F = -Nk_BT\left[1 + \log\frac{(V-Nb')T^{3/2}}{Nc'}\right] - \frac{a'N^2}{V}$$

$\beta P = \rho$

- Critical Point of Van der Waals Model.

$$P = \frac{k_B T}{V-b} - \frac{a}{V^2} \quad (*)$$



$\{V_L, V_1, V_2, V_G\} \to \{V_c\}$.

(At $T = T_c$).

① $\partial P/\partial V \big|_{V_c} = 0$
② $\partial^2 P/\partial V^2 \big|_{V_c} = 0$
$\Big\}$ Inflection point!

① $\partial P/\partial V = -k_B T \cdot (V_c - b)^{-2} + 2a V_c^{-3} = 0$

$$\Rightarrow \quad 2a V_c^{-3} = k_B T_c (V_c - b)^{-2}$$

② $\partial^2 P/\partial V^2 = 2k_B T (V_c - b)^{-3} - 6a V_c^{-4} = 0$

$$\Rightarrow \quad 6a V_c^{-4} = 2k_B T_c (V_c - b)^{-3}$$

$$\Rightarrow \tfrac{1}{3} \cdot V_c^{+1} = \tfrac{1}{2} \cdot (V_c - b)^{+1} \Rightarrow 3V_c - 3b = 2V_c \Rightarrow \underline{V_c = 3b}$$

(*) $\Rightarrow P_c = \frac{k_B T_c}{2b} - \frac{a}{9b^2}$

① $\Rightarrow 2a(3b)^{-3} = k_B T_c \cdot (2b)^{-2} \Rightarrow \underline{k_B T_c = \frac{8a}{27b}}, \quad \underline{P_c = \frac{a}{27b^2}}$

- Non-dimensional variables

$\hat{P} = P/P_c, \quad \hat{V} = V/V_c, \quad \hat{T} = T/T_c.$

$$\Rightarrow \hat{P} \cdot P_c = \frac{k_B \hat{T} \cdot T_c}{\hat{V} \cdot V_c - b} - \frac{a}{(\hat{V} \cdot V_c)^2}$$

$$\Rightarrow \hat{P} \cdot \frac{\cancel{a}}{27\cancel{b^2}} = \frac{\frac{8\cancel{a}}{27\cancel{b}} \hat{T}}{3\cancel{b}\hat{V} - \cancel{b}} - \frac{\cancel{a}}{(3\cancel{b}\hat{V})^2}$$

$$\frac{\hat{P}}{27} = \frac{8\hat{T}/27}{3\hat{V} - 1} - \frac{1}{9\hat{V}^2}$$

$$\Rightarrow \underline{\left(\hat{P} + \frac{3}{\hat{V}^2}\right)\left(3\hat{V} - 1\right) = 8\hat{T}}$$

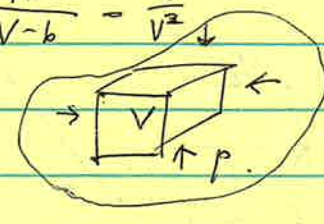
(*')

- Critical Exponent (κ_T)

Given $(\hat{p} + 3/\hat{v}^2)\cdot(3\hat{v} - 1) = 8\hat{T}$. $\Leftrightarrow$ $p = \frac{k_B T}{V-b} - \frac{a}{V^2}$

Q1) what happens $\hat{v} \approx 1/3$ $\Leftrightarrow$ $V \approx \frac{1}{3} V_c$

Q2) Isothermal compressibility $\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial p}$



$k_T = -\frac{1}{V} \cdot \partial V / \partial p$.

→ watch $\partial p / \partial V = -k_B T \cdot (V-b)^{-2} + 2a V^{-3}$

→ $\partial V / \partial p = \frac{1}{-k_B T (V-b)^{-2} + 2aV^{-3}}$ $\Rightarrow$ $k_T = \frac{1}{k_B T \cdot V (V-b)^{-2} - 2aV^{-2}}$

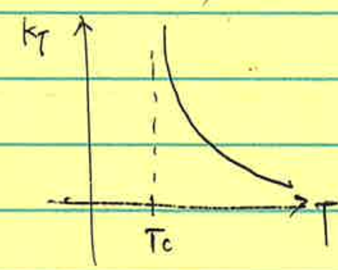
→ Around $T = T_c$, $V = V_c = 3b$

$$k_T = \frac{1}{k_B T \cdot 3b (2b)^{-2} - 2a (3b)^{-2}}$$

(and apply $a = \frac{27}{8} b\, k_B T_c$)

$$\Rightarrow k_T = \frac{1}{\frac{3k_B}{4b} T - \frac{3k_B}{4b} T_c} = \frac{4b}{3k_B}(T - T_c)^{-1}$$

$\boxed{\gamma = 1}$



- Critical Exponent (V) $T \to T_c$

Q) How does volume deviate around T_c ?

We know non-dimensional relation.

$$\hat{p} = \frac{8\hat{T}}{3\hat{V} - 1} - \frac{3}{\hat{V}^2} \qquad \left\{ \begin{array}{l} \hat{T} \to 1 + \delta\hat{T} \\ \hat{V} \to 1 + \delta\hat{V} \end{array} \right\}$$

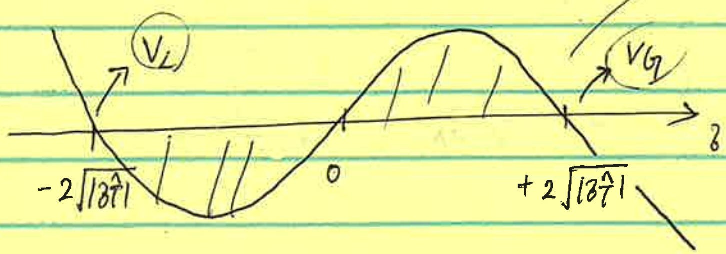
$4(1+\delta\hat{T})$ $\quad$ 3

$$\hat{p} = \frac{8(1+\delta\hat{T})}{2 + 3\delta\hat{V}} - \frac{3}{(1+\delta\hat{V})^2} = \frac{4(1+\delta\hat{T})}{1+\frac{3}{2}\delta\hat{V}} - \frac{3}{(1+\delta\hat{V})^2}$$

$\approx 1 + 4\delta\hat{T}$

$$\Rightarrow \hat{p} \approx 1 + 4\delta\hat{T} - 6(\delta\hat{T})(\delta\hat{V})\left(1 + \frac{(\delta\hat{V})^2}{4\delta\hat{T}}\right).$$

Maxwell's construction (convexity).



$$\Rightarrow \underline{\delta\hat{v} = \pm 2\sqrt{|\delta\hat{\tau}|}}$$

$(T < T_c \text{ and } \hat{\tau} < 1)$

$$\Rightarrow \hat{v} = 1 \pm 2\sqrt{1-\hat{\tau}} \Rightarrow \hat{v} = V/V_c = 1 \pm 2\sqrt{1-T/T_c}$$

$$\Rightarrow V_G - V_L = 4V_c\left(1 - T/T_c\right)^{1/2} = 12b \cdot \left(1 - T/T_c\right)^{1/2}$$

Thus, $V_G - V_L$ goes to zero following $\propto (T_c - T)^{1/2}$

$$= (T_c - T)^{\tilde{\beta}}$$

$\underline{\tilde{\beta} = 1/2}$

- Problem Session (ME346A) 03/08/2025
- <u>Monte Carlo</u> Simulation (Rosenbluth, Teller, Metropolis)

  at Markov chain.

  ① Initial state ν

  ② Generate random state ν'

  ③ Evaluate probability

  $$\frac{p(\nu')}{p(\nu)} = \frac{\frac{1}{Z}\cdot e^{-\beta E(\nu')}}{\frac{1}{Z}\cdot e^{-\beta E(\nu)}} = e^{-\beta\{E(\nu')-E(\nu)\}} = e^{-\beta\Delta E}$$

  ④ Accept / reject with probability,

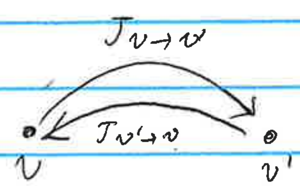
  $$p_{acc}(\nu\to\nu') = \min\left(1,\ e^{-\beta\Delta E}\right).$$

- <u>Detailed Balance.</u>

  $$p(\nu)\cdot p(\nu\to\nu') = p(\nu')\,p(\nu'\to\nu)$$

  $$\Leftrightarrow\quad \frac{p(\nu\to\nu')}{p(\nu'\to\nu)} = \frac{p(\nu')}{p(\nu)}$$

  Note: $\underbrace{p(\nu)}\cdot\underbrace{p(\nu\to\nu')} \simeq$ "flux."



  If you select any pairs of ν and ν', (ν, ν')

  Fluxes $J_{\nu\to\nu'} = J_{\nu'\to\nu}$

  Global detailed balance $\to$ No net flow

  No net flow $\to$ Reversible.

  Reversible $\to$ Equilibrium distribution is sampled.

- Examine detailed balance for MCMC.

$$P(\nu \to \nu') = \underbrace{P_{gen}(\nu \to \nu')}_{\text{probability to generate such move}} \cdot \underbrace{P_{acc}(\nu \to \nu')}_{\text{probability to accept such move.}}$$

From detailed balance,

$$\frac{P(\nu)}{P(\nu')} = \frac{P(\nu' \to \nu)}{P(\nu \to \nu')} = \frac{P_{gen}(\nu' \to \nu) \cdot P_{acc}(\nu' \to \nu)}{P_{gen}(\nu \to \nu') \cdot P_{acc}(\nu \to \nu')}$$

when generating (proposing) probabilites are "symmetric", (i.e. $P_{gen}(\nu \to \nu') = P_{gen}(\nu' \to \nu)$)

$$\frac{P(\nu)}{P(\nu')} = \frac{P_{acc}(\nu' \to \nu)}{P_{acc}(\nu \to \nu')}$$

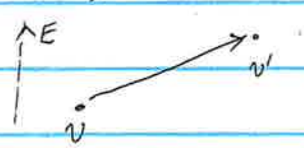
Metropolis–Hastings.

Apply Monte carlo, where $\boxed{P_{acc}(\nu \to \nu') = \min\left[1, e^{-\beta \Delta E}\right]}$ $\left(\Delta E = E(\nu') - E(\nu)\right)$

$$\frac{p(\nu' \to \nu)}{p(\nu \to \nu')} = \frac{P(\nu)}{P(\nu')} = \frac{\min\left[1, e^{+\beta\Delta E}\right]}{\min\left[1, e^{-\beta \Delta E}\right]} \overset{\text{should be,}}{=} \frac{e^{-\beta E(\nu)}}{e^{-\beta E(\nu')}} = e^{+\beta(E(\nu') - E(\nu))}$$

$$= \underbrace{e^{\beta \Delta E}}_{\text{Condition for D.B.}}$$

Case 1) $\Delta E > 0$

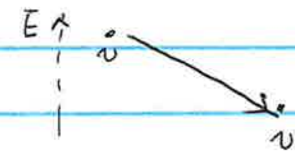


$\min\left[1, e^{-\beta\Delta E}\right] = e^{-\beta\Delta E}$

$\min\left[1, e^{+\beta\Delta E}\right] = 1$

$P(\nu)/P(\nu') = e^{+\beta\Delta E}$

Case 2) $\Delta E < 0$



$\min\left[1, e^{-\beta\Delta E}\right] = 1$

$\min\left[1, e^{+\beta\Delta E}\right] = e^{\beta\Delta E}$

$P(\nu)/P(\nu') = e^{\beta\Delta E}$.

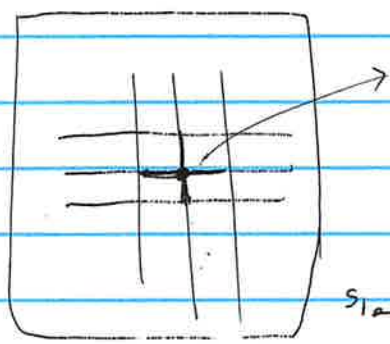
Some notes on Monte Carlo.

① How do you implement it?

Main question : How to probability

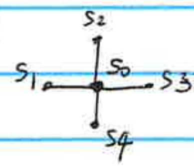
EX) np. random.rand() < 0.3

② How to calculate energy difference in Ising Model?



(i, j)

$$H = -J\sum_{\langle i,j\rangle} s_i s_j - h\sum_i s_i$$



Before : $-h s_0 - h s_1 \cdots - h s_4$

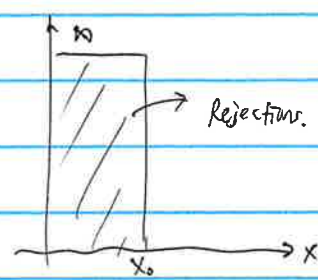
After : $+h s_0 - h s_1 \cdots - h s_4$.

Before : $-J\, s_0 s_1 - J \cdot s_0 s_3 - J s_0 s_2 - J s_0 s_4$

After : $-J(-s_0) s_1 - J(-s_0) s_3 - J(-s_0) s_2 - J(-s_0) s_4$

$$\Delta H = -h(-s_0 - s_0) - J(s_1 + \cdots + s_4) \cdot (-s_0 - s_0)$$
$$= 2\left(-h \cdot s_0 - J \cdot s_0 (s_1 + \cdots + s_4)\right)$$

③ Hard disk model



[1] Equation of State Calculations by Fast Computing Machines. (1953)

$\cdot\ F_i = m \cdot \ddot{q}$ (1687)

$\dfrac{dp_i}{dt} = F_i$ ——— ①

$\cdot\ \mathcal{L} = K - U = \sum_i \frac{1}{2} m (\dot{q}_i)^2 - U(q_i)$

$\dfrac{d}{dt}\left(\partial L / \partial \dot{q}_i\right) - \partial L / \partial q_i = 0 \quad \forall_i$ (1760) ——— ②

$\dfrac{d}{dt}(m\dot{q}) + \left(+\dfrac{\partial}{\partial q_i} U(q_i)\right) = 0$

$\Rightarrow \ddot{q} = -\dfrac{1}{m} \nabla U(q)$

$\ddot{q}_i = -\dfrac{1}{m}\dfrac{\partial U}{\partial q_i} \sim ①$

$$\frac{dL}{dt} = \sum_i \underbrace{\frac{\partial L}{\partial q_i}\frac{dq_i}{dt}}_{(1)} + \underbrace{\frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt}}_{(2)}$$

$$(2) = \frac{dL}{d\dot{q}_i}\frac{d}{dt}(\dot{q}_i)$$

$$(1) = \frac{\partial L}{\partial q}\frac{dq}{dt} = \frac{\partial \dot{q}_i}{\partial q_i}\frac{\partial L}{\partial \dot{q}_i}\frac{dq}{dt} \quad \dot{q}$$

$$= \frac{d}{dt}\underbrace{\left(\partial L / \partial \dot{q}_i\right)}_{u}\underbrace{\dot{q}_i}_{v}$$

$$\Rightarrow \frac{d}{dt}\left[\frac{\partial L}{\partial q_i}\dot{q}_i\right] + \frac{dL}{d\dot{q}_i}\frac{d}{dt}\left[\dot{q}_i\right]$$

$(uv)' = u'v + uv'$

$$\Rightarrow \frac{dL}{dt} = \frac{d}{dt}\left[\underbrace{\frac{\partial L}{\partial \dot{q}_i}}_{u}\underbrace{\dot{q}_i}_{v}\right] \Rightarrow \frac{d}{dt}\left[\underbrace{-L + \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i}_{H}\right] = 0$$

$$H = -L + \underbrace{\frac{\partial L}{\partial \dot{q}_i}}_{=p_i}\dot{q}_i = -L + p_i\dot{q}_i$$

Ex) $H = \dfrac{p^2}{2m} + U(x) \quad H(\dot{x}, p)$

m

$p = mv$

$L = -H + \left(\dfrac{\partial H}{\partial p}\right)p = -H + v \cdot p$

① $dH = \dfrac{\partial H}{\partial p}dp + \dfrac{\partial H}{\partial x}dx = v\,dp + U'(x)\,dx$

② $dL = -dH + v\,dp + p\,dv = \cancel{-v\,dp} - U'(x)\,dx + \cancel{v\,dp} + p\,dv$

$L(x, v)$

$H = -L + \left(\dfrac{\partial L}{\partial v}\right)v$

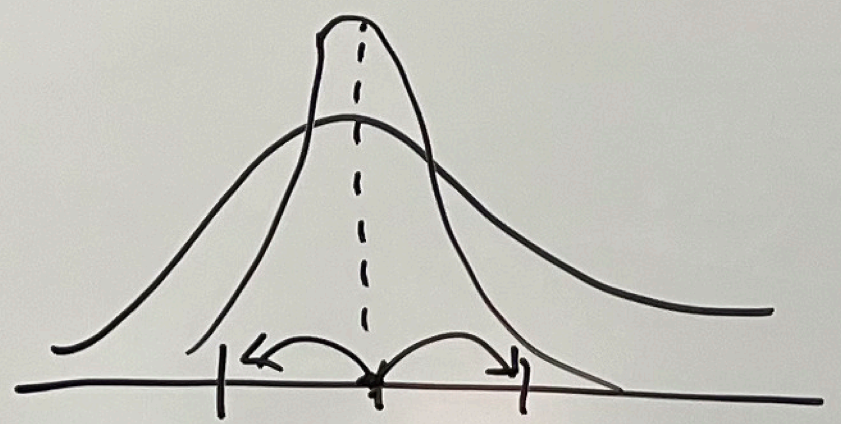
$\boxed{\text{Quiz}}$ 01/17/2025

- If RVs X, Y satisfy $\langle XY \rangle = \langle X \rangle \langle Y \rangle$, they are independent. F

  0 0

- $J = \frac{N_{net}}{\text{Area} \cdot \text{Time}}$ T

- $l_i = \pm 1$ prob : $p = 1/2$; 0 prob : $1-2p$ — $l_i = \pm 1$ prob : $1/2$ F

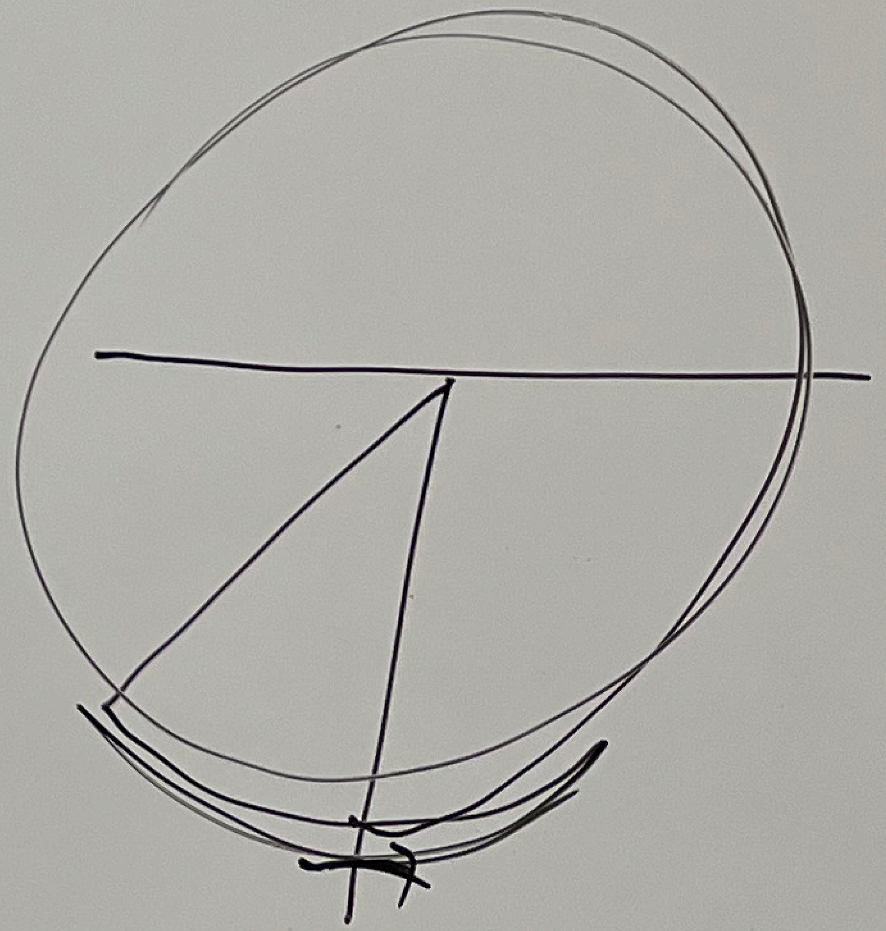


$Y = X^2$

$X = [-1, +1]$

$P(Y=y \mid X=x) = P(Y=y)$

- $L = K - U$, L is conserved. F



- U is conservative field. $dH/dt = 0 \Rightarrow$ Conservation of energy. T

  ∇

- $F_i = m \cdot \ddot{q}$ (1687)

$\underbrace{\frac{dp_i}{dt} = F_i}$ —— ①

- $\mathcal{L} = K - U = \sum_i \frac{1}{2} m (\dot{q}_i)^2 - U(q_i) - \xi(\dot{q})q$

$\underbrace{\frac{d}{dt}\left(\partial L / \partial \dot{q}_i\right) - \partial L / \partial q_i = 0} \quad \forall_i$ (1760) —— ②

$$\frac{d}{dt}(m\dot{q}) + \left(+\frac{\partial}{\partial q_i} U(q_i)\right) = 0$$

$$\Rightarrow \ddot{q} = -\frac{1}{m} \nabla U(q)$$

$$\ddot{q}_i = -\frac{1}{m} \frac{\partial U}{\partial q_i} \sim ①$$

$$\underset{\text{LHS}}{\frac{dL}{dt}} = \sum_i \underbrace{\frac{\partial L}{\partial q_i}\frac{dq_i}{dt}}_{(1)} + \underbrace{\frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt}}_{(2)}$$

$$= \frac{dL}{d\dot{q}_i}\frac{d}{dt}(\dot{q}_i)$$

$$(1) = \sum \frac{\partial L}{\partial q_i}\frac{dq_i}{dt} = \sum \frac{\partial \dot{q}_i}{\partial \dot{q}_i}\frac{\partial L}{\partial q_i}\frac{dq}{dt} \quad \dot{q}$$

$$= \sum \frac{d}{dt}\big(\underbrace{\partial L / \partial \dot{q}_i}_{u}\big)\underbrace{\dot{q}_i}_{v}$$

$$\Rightarrow \underbrace{\sum \frac{d}{dt}\left[\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i\right]}_{(1)} + \underbrace{\frac{dL}{d\dot{q}_i}\frac{d}{dt}[\dot{q}_i]}_{(2)} \quad \text{RHS}$$

$$\Rightarrow \underset{\text{LHS}}{\frac{dL}{dt}} = \underset{\text{RHS}}{\sum \frac{d}{dt}\left[\underbrace{\frac{\partial L}{\partial \dot{q}_i}}_{u}\underbrace{\dot{q}_i}_{v}\right]} \Rightarrow \frac{d}{dt}\Big[\underbrace{-L + \sum \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i}_{H}\Big] = 0$$

$$\begin{cases} \frac{\partial L}{\partial \dot{q}_i} = p_i & \frac{\partial L}{\partial q_i} = \frac{\partial \dot{q}_i}{\partial q_i}\underbrace{\frac{\partial L}{\partial \dot{q}_i}} = \frac{d}{dt}p_i = \dot{p}_i \\ \frac{\partial L}{\partial q_i} = \dot{p}_i \end{cases}$$

EOM L

EOM H

$$\begin{cases} \frac{\partial H}{\partial p} = \dot{q} \\ \frac{\partial H}{\partial q} = -\dot{p} \end{cases}$$

$$H = -L + p\dot{q}$$

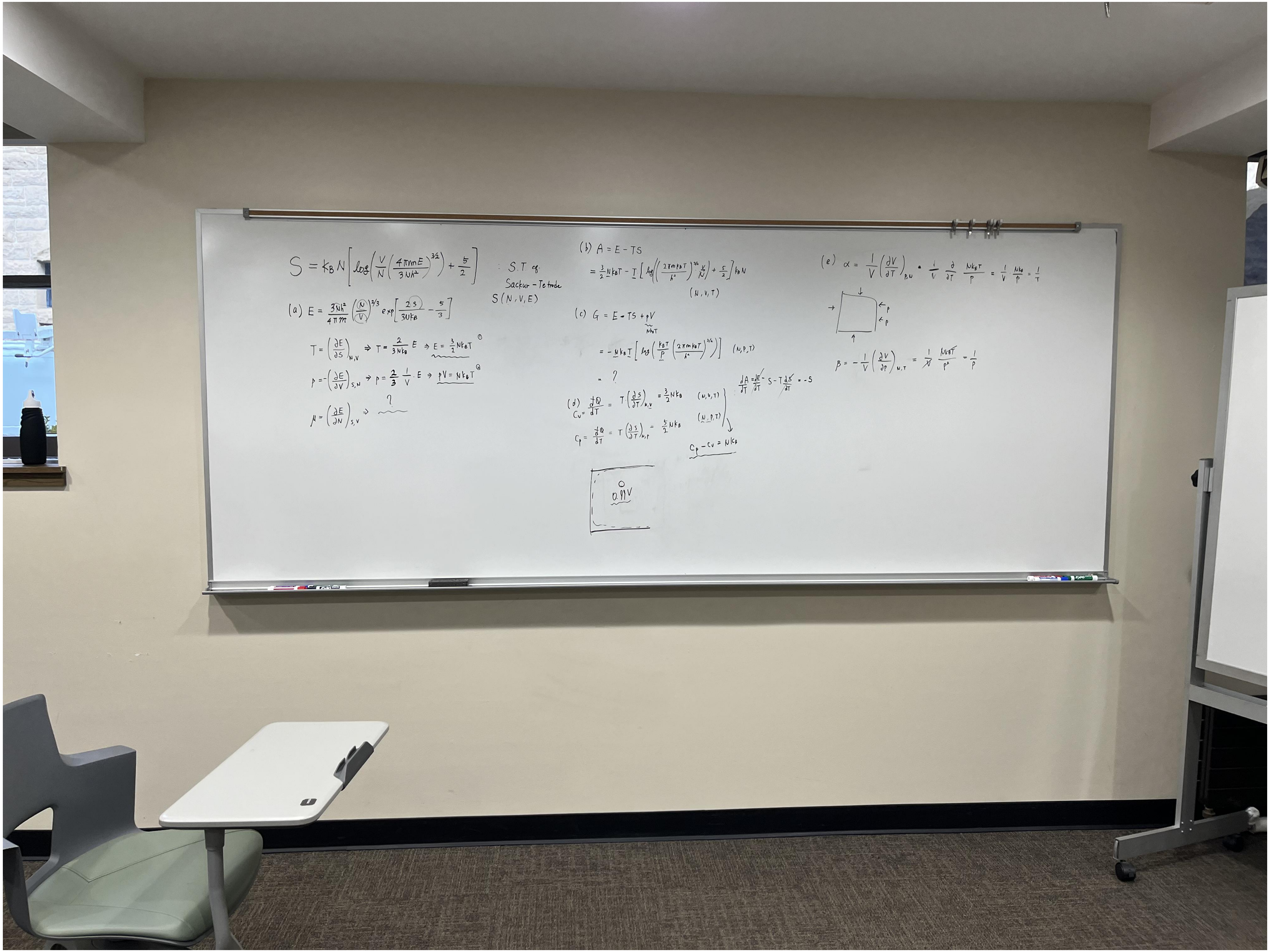
$$dH = dp\,\dot{q} + \cancel{d\dot{q}\,p} - \underbrace{\frac{\partial L}{\partial \dot{q}}d\dot{q}}_{\cancel{p\,d\dot{q}}} - \underbrace{\frac{\partial L}{\partial q}dq}_{\dot{p}\,dq} = \underbrace{\dot{q}}_{\frac{\partial H}{\partial p}}dp - \underbrace{\dot{p}}_{\frac{\partial H}{\partial q}}dq$$

① $L \leftrightarrow H$

② $dH/dt = 0$

$$e^{-\beta U}$$

$$U \in C^\infty$$



$S = k_B N \left[\log\left(\frac{V}{N} \left(\frac{4\pi m E}{3Nh^2} \right)^{3/2} \right) + \frac{5}{2} \right]$
: S.T eq.
Sackur - Tetrode
$S(N, V, E)$
(a) $E = \frac{3Nh^2}{4\pi m} \left(\frac{N}{V} \right)^{2/3} \exp\left[\frac{2S}{3Nk_B} - \frac{5}{3} \right]$
$T = \left(\frac{\partial E}{\partial S} \right)_{N,V} \Rightarrow T = \frac{2}{3Nk_B} E \Rightarrow E = \frac{3}{2} N k_B T$ ①
$p = -\left(\frac{\partial E}{\partial V} \right)_{S,N} \Rightarrow p = \frac{2}{3} \frac{1}{V} \cdot E \Rightarrow pV = N k_B T$ ②
$\mu = \left(\frac{\partial E}{\partial N} \right)_{S,V} \Rightarrow$?
(b) $A = E - TS$
$= \frac{3}{2} N k_B T - T \left[\log\left(\left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} \frac{V}{N} \right) + \frac{5}{2} \right] k_B N$
(N, V, T)
(c) $G = E - TS + \underbrace{pV}_{Nk_BT}$
$= -N k_B T \left[\log\left(\frac{k_B T}{P} \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} \right) \right]$ (N, P, T)
$= ?$
$\frac{dA}{dT} = \cancel{\frac{dE}{dT}} - S - T \cancel{\frac{dS}{dT}} = -S$
(d) $C_V = \frac{đQ}{dT} = T \left(\frac{\partial S}{\partial T} \right)_{N,V} = \frac{3}{2} N k_B$ (N, V, T)
$C_p = \frac{đQ}{dT} = T \left(\frac{\partial S}{\partial T} \right)_{N,P} = \frac{5}{2} N k_B$ (N, P, T)
$C_p - C_V = N k_B$
0.99V
(e) $\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_{P,N} = \frac{1}{V} \frac{\partial}{\partial T} \frac{N k_B T}{P} = \frac{1}{V} \cdot \frac{N k_B}{P} = \frac{1}{T}$
P
P
$\beta = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_{N,T} = \frac{1}{\cancel{V}} \frac{\cancel{N k_B T}}{P^2} = \frac{1}{P}$

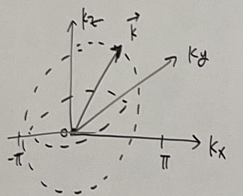
$$Z = \sum_{\nu} e^{-\beta E(\nu)} \approx \int dE\, \Omega(E)\, e^{-\beta E(\nu)} \qquad \text{Laplace}$$

$$= \int dE\, e^{-\beta[\underbrace{E(\nu) - \log\Omega(E)}_{=A(\nu)}]} \qquad \text{Legendre}$$

Ω	E
Z	A
Ξ	G
Δ	?
$T\ P$	

- **Density of States.**

$\vec{k}$: wave vector.



$\vec{k} = \left(\frac{2\pi}{L}\right)(n_x, n_y, n_z)$ $\qquad \frac{2\pi}{L}\cdot n = \frac{2\pi}{(L/n)}$ λ

$g(k)\,dk = \frac{4\pi k^2\,dk}{(2\pi/L)^3} = \frac{L^3}{2\pi^2}\cdot k^2$

$e^{-\beta\hbar\omega}$

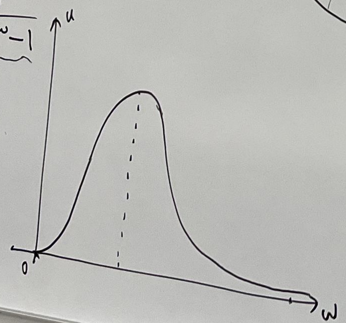
- **Planck's law** $\cancel{\mu=0}$

$u \propto 2\,\varepsilon(\omega)\cdot g(\omega)\,d\omega\cdot\langle n_i\rangle_B = \frac{1}{e^{\beta\hbar\omega}-1}\cdot\omega\cdot\omega^2\,d\omega$

$\propto \frac{\omega^3}{e^{\beta\hbar\omega}-1}$

$\omega\to 0 \quad u\propto\omega^2 \to$ Rayleigh-Jeans law.

$\omega\to\infty \quad u\to 0$

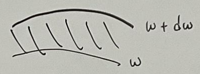


- **photons**

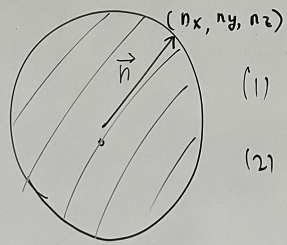
ⓔ ↑↓ ⓟ : polarization.

$\omega = 2\pi f$

$g(\omega)\,d\omega = \frac{\partial N(\omega)}{\partial\omega}\cdot d\omega$



$g(k)\,dk = \frac{\partial N(k)}{\partial k}\,dk.$



(1) $N = \frac{4}{3}\pi\|\vec{n}\|^3 \propto \|P\|^3 \propto \|\varepsilon\|^3 \propto \omega^3 \to g(\omega)\,d\omega \propto \omega^2\,d\omega$

(2) $4\pi\|\vec{n}\|^2\cdot d\|\vec{n}\| \propto \omega^2\,d\omega = g(\omega)\,d\omega$

$g(\omega)\,d\omega \propto \omega^2\,d\omega$

- $p = \frac{h}{\lambda} = \frac{hf}{c} \Rightarrow pc = \varepsilon$

- $k = \frac{2\pi}{\lambda}$ $\qquad$ - $\varepsilon = hf = \hbar\omega$

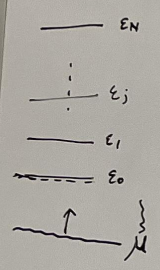
- $\boxed{p = \hbar k}$

$\|P\| \propto \hbar\,\|\vec{n}\|$

$\Rightarrow \|\vec{n}\| \propto \|P\|$

· Grand Canonical Ensemble.

$$\mathcal{Z}_{Boson} = \sum_{n_0=0}^{\infty}\sum_{n_1=0}^{\infty}\cdots\sum_{n_N=0}^{\infty} e^{-\beta\left(\sum_j n_j \varepsilon_j - \mu \sum_j \varepsilon_j\right)}$$



$$= \prod_{j=0}^{N} \underbrace{\sum_{n}^{\infty} e^{-\beta(\varepsilon_j-\mu)n}} \rightarrow \frac{1}{1-e^{-\beta(\varepsilon_j-\mu)}}$$

$$\left(\sum_{n=0}^{\infty} r^n = \frac{1}{1-r} \qquad |r|<1 \right)$$

$$-\beta(\varepsilon_j-\mu) < 0 \rightarrow \varepsilon_j > \mu$$

$$\underline{\varepsilon_0 > \mu}$$

μVT

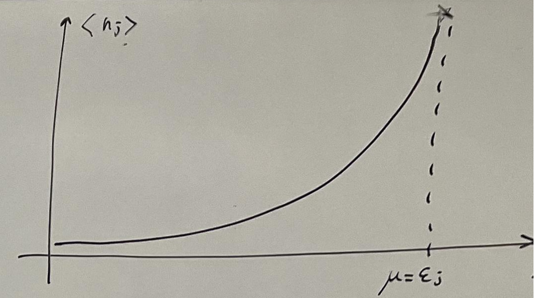
$$\boxed{\begin{aligned} \mathcal{Z}_B &= \prod_{j=0}^{N} \frac{1}{1-e^{-\beta(-\mu+\varepsilon_j)}} \\ \mathcal{Z}_F &= \prod_{j=0}^{N} 1+e^{-\beta(\varepsilon_j-\mu)} \end{aligned}}$$

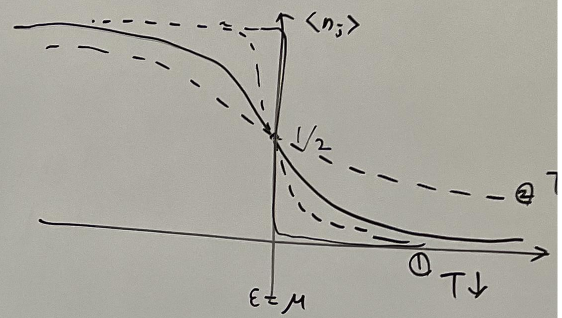
$$\langle n_j \rangle_{Bosons} = \frac{\partial \log \mathcal{Z}_B}{\partial(-\beta(\varepsilon_j-\mu))} = \frac{1}{e^{\beta(\varepsilon_j-\mu)}-1}$$

$$\Delta n_j\ {}_{Bosons} = \frac{\partial^2 \log \mathcal{Z}_B}{\partial(-\beta(\varepsilon_j-\mu))^2}$$

$$\langle n_j \rangle_{Fermion} = \frac{1}{e^{\beta(\varepsilon_j-\mu)}+1} \qquad \Delta n_{j\ F}. \qquad \beta = \frac{1}{k_B T}$$

$$\rightarrow \frac{\partial . \log Z}{\partial(-\beta)} = \underset{\sim}{\frac{1}{Z}} \frac{\partial Z}{\partial(-\beta)}$$





critical phenomena

$$\hat{p} = p/p_c$$
$$\hat{V} = V/V_c$$
$$\hat{T} = T/T_c$$

$$\rightarrow \left(\hat{p} + \frac{3}{\hat{V}^2}\right)\cdot\left(3\hat{V} - 1\right) = 8\hat{T}$$

$$\frac{\partial p}{\partial V} = -k_B T (V-b)^{-2} + 2a V^{-3}$$

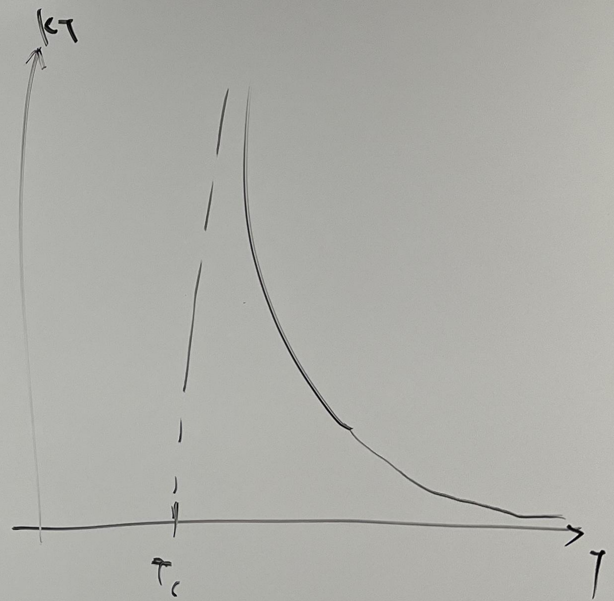
$$k_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T$$

$$\frac{\partial V}{\partial p} = \frac{1}{-k_B T (V-b)^{-2} + 2a V^{-3}}$$

$$k_T = -\frac{1}{V}\frac{\partial V}{\partial p} = \frac{1}{k_B T \cdot V (V-b)^{-2} - 2a V^{-2}}$$

$$= \frac{4b}{3k_B}\left(T - T_c\right)^{-1} \quad T > T_c$$

$\alpha = 1$



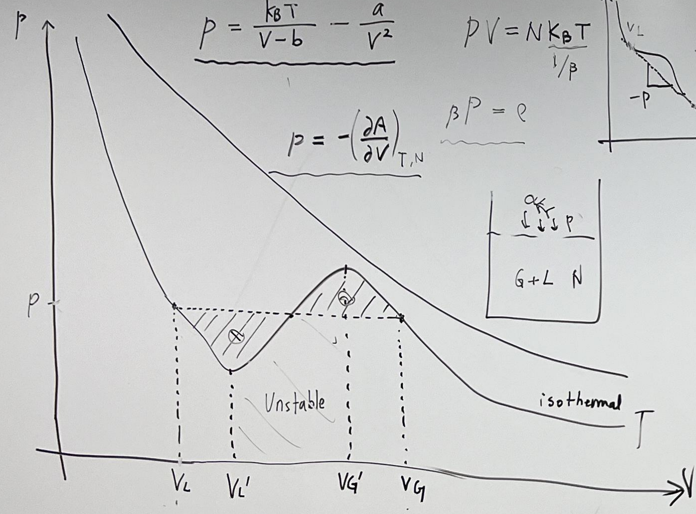
Van der Waals Model

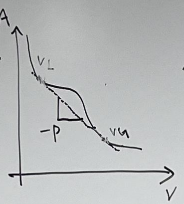
$$p = \frac{k_B T}{V-b} - \frac{a}{V^2}$$

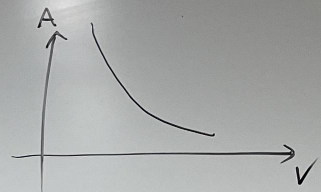
$$pV = N k_B T \qquad k_B T = 1/\beta$$

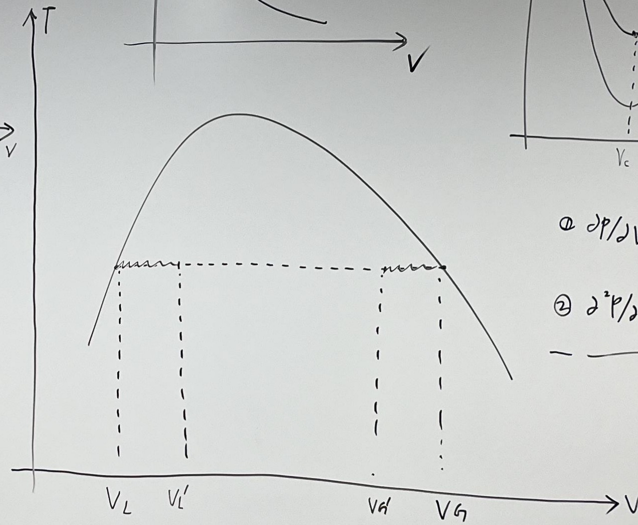
$$p = -\left(\frac{\partial A}{\partial V}\right)_{T,N}$$

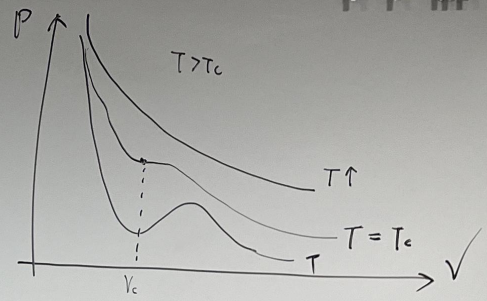
$$\beta P = \rho$$







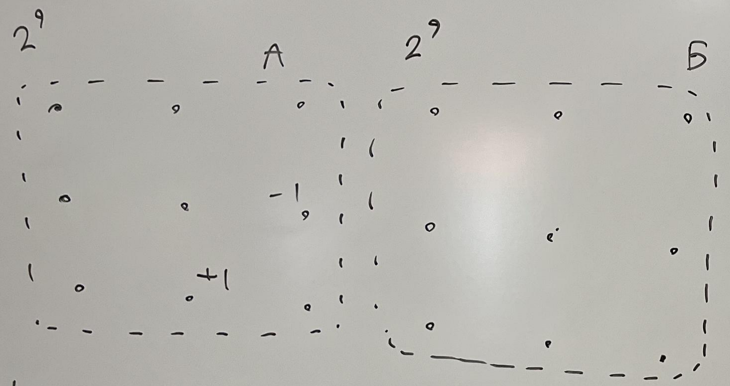


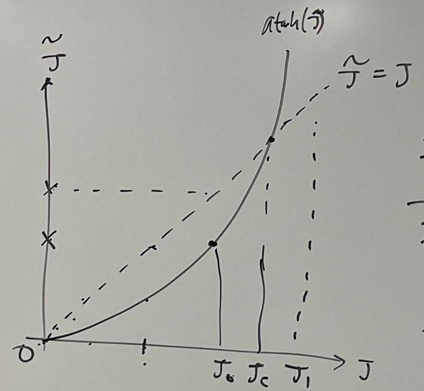


① $\left.\partial p/\partial V\right|_{V_c} = 0 \Rightarrow 2aV_c^{-3} = k_B T_c (V_c - b)^{-2}$

② $\left.\partial^2 p/\partial V^2\right|_{V_c} = 0 \Rightarrow 6aV_c^{-4} = 2k_B T_c (V_c - b)^{-3}$

$$\boxed{V_c = 3b \qquad k_B T_c = \frac{8a}{27b} \qquad p_c = \frac{a}{27b^2}}$$





18 spins $= 2^{18}$

$$\sigma_A = \begin{cases} +1 & \sum_{i,j \in A} > 0 \\ -1 & \text{"} \quad < 0 \end{cases}$$

$$Z = \sum_{\sigma_A, \sigma_B} \tilde{Z}(\sigma_A, \sigma_B)$$

$$\tilde{Z} = e^{-\beta \tilde{H}} \qquad \tilde{H} = -\tilde{J}\sigma_A \sigma_B - C - \tilde{h}\sigma_A - \tilde{h}\sigma_B$$

} MATH.

$$\beta \tilde{J} = \operatorname{arctanh}(\beta J)$$

$$\begin{pmatrix} \tilde{Z}_{+1,+1} & \tilde{Z}_{+1,-1} \\ \tilde{Z}_{-1,+1} & \tilde{Z}_{-1,-1} \end{pmatrix} = e^{\beta c} \begin{pmatrix} e^{\beta \tilde{J} + \beta 2h} & e^{-\beta \tilde{J}} \\ e^{-\beta \tilde{J}} & e^{\beta \tilde{J} - \beta 2h} \end{pmatrix}$$

$$\frac{Z_{+1,+1} - Z_{+1,-1}}{Z_{+1,+1} + Z_{+1,-1}} = \frac{e^{\beta \tilde{J} + \beta h} - e^{-\beta \tilde{J} - \beta h}}{e^{\beta \tilde{J} + \beta h} + e^{-\beta \tilde{J} - \beta h}} = \tanh(\underbrace{\beta \tilde{J} + \beta h}_{\tilde{J}}) = \beta J + \beta h$$

$\tilde{J}$

· Monte Carlo

① ν

② ν' $\quad \Delta E$

③ $$\frac{P(\nu')}{P(\nu)} = \frac{e^{-\beta E(\nu')}}{e^{-\beta E(\nu)}} = e^{-\beta\{E(\nu')-E(\nu)\}} = e^{-\beta\Delta E}$$

④ Accept / Reject

$$\underbrace{P_{acc}(\nu\to\nu') = \min[1, e^{-\beta\Delta E}]}_{\text{Metropolis - Hastings.}} = 0.1$$

· Detailed Balance ≡ No net flow

↓

· Equilibrium. ← Reversible

$$\underbrace{P(\nu)\cdot P(\nu\to\nu')}_{\simeq \text{Flux}} = P(\nu')\cdot P(\nu'\to\nu)$$

· $P(\nu\to\nu') = P_{gen}(\nu\to\nu')\,P_{acc}(\nu\to\nu')$

$\qquad \| $

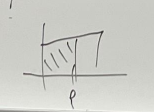
$\quad P_{gen}(\nu'\to\nu)$ (if symmetric)

Python - How to prob.

~~import numpy as np~~

$[0,1]$ $1/6$ $P<1$

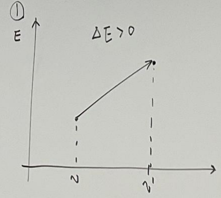
if np.random.rand() < P



· D.B for M.C.

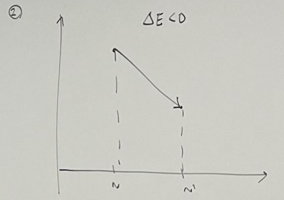
$$\frac{P(\nu')}{P(\nu)} = \frac{P(\nu\to\nu')}{P(\nu'\to\nu)} = \frac{\min(1, e^{-\beta\Delta E})}{\min(1, e^{+\beta\Delta E})}$$

① $\Delta E > 0$



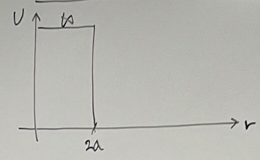
$$\frac{P(\nu')}{P(\nu)} = \frac{e^{-\beta\Delta E}}{1} = e^{-\beta\Delta E}$$

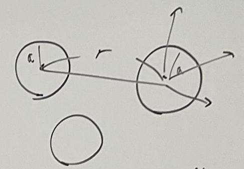
② $\Delta E < 0$



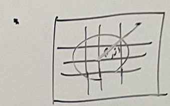
$$\frac{P(\nu')}{P(\nu)} = \frac{1}{e^{\beta\Delta E}} = e^{-\beta\Delta E}$$

· Notes





$$|r_{ij} - r_{i'j'}|^{-P}$$



PF3.

$\vec{k} = (k_x, k_y, k_z) = \frac{2\pi}{L}(n_x, n_y, n_z)$ $E_0 = mc^2$

$E = (p^2c^2 + \underbrace{m^2c^4}_{E_0^2})^{1/2}$ $\vec{p} = \hbar\vec{k}$ $p^2c^2 = \hbar^2k^2c^2$ $p^2 = \hbar^2k^2$

(a) $g(E)$

(b) $E - E_0 \ll E_0$

(c) $E - E_0 \gg E_0$

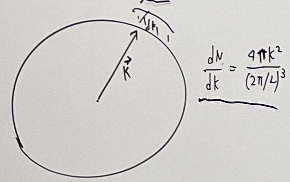
$E^2 - E_0^2 = \hbar^2k^2c^2$ —— (1)

$\cancel{2}E\,dE = \cancel{2}\hbar^2c^2\,k\,dk$

$dE/dk = \frac{\hbar^2c^2}{E}k$ $\rightarrow dk/dE = \frac{E}{\hbar^2c^2}\frac{1}{k}$

$g(E)\,dE = dN$

$g(E) = \frac{dN}{dE} = \frac{dN}{dk}\cdot\frac{dk}{dE}$



$\frac{dN}{dk} = \frac{4\pi k^2}{(2\pi/L)^3}$

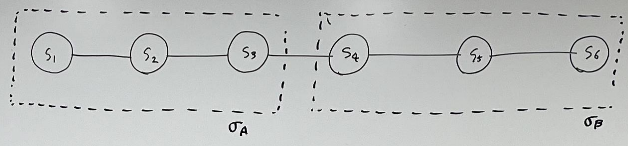
$\therefore g(E) \propto E\sqrt{E^2-E_0^2}$

$dN = 4\pi k^2\,dk\cdot\left(\frac{L}{2\pi}\right)^3$

$N = \underbrace{\frac{4}{3}\pi k^3}_{V}\left(\frac{L}{2\pi}\right)^3$

$N = \frac{4}{3}\pi n^3$

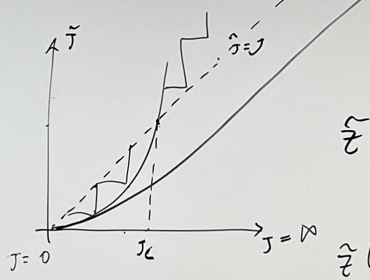
PF5.



$H = -J\sum_{\langle i,j\rangle} s_i s_j$ $(h=0)$

$\sigma_A = \begin{cases} +1 & s_1+s_2+s_3>0 \\ -1 & s_1+s_2+s_3<0 \end{cases}$

$\sigma_B = \begin{cases} +1 & s_4+s_5+s_6>0 \\ -1 & s_4+s_5+s_6<0 \end{cases}$



(Q) Find J_c

$\tilde H = -\tilde J\sigma_A\sigma_B - C$

1) +1	+1	→ 16	
+1	−1	→ 16	
−1	+1	→ 16	$\sum_{\{s_i\}} z$
−1	−1	→ 16	

$\tilde Z(\sigma_A = +1, \sigma_B = +1)$ ||

$\tilde Z(+1,+1) = \sum_{\{s_i\}} Z(s_1 \sim s_6)$

$\beta\tilde J$ βJ

$\tilde Z(+1,-1) =$?

$\tilde J = f(J)$

J_c

3-(b) $E - E_0 << E_0$

$$g(E) \propto E\sqrt{E^2 - E_0^2} = E\sqrt{(E-E_0)\underbrace{(E+E_0)}}$$

$$E = \{p^2c^2 + m^2c^4\}^{1/2} = E_0\left(1 + \left(\frac{pc}{E_0}\right)^2\right)^{1/2} = E_0\left(1 + \frac{1}{2}\left(\frac{pc}{E_0}\right)^2\right) = E_0\left(1 + \frac{1}{2}\left(\frac{pc}{mc^2}\right)^2\right) = E_0\left(1 + \frac{1}{2}\cdot\left(\frac{p}{mc}\right)^2\right)$$

$$E = E_0\left(1 + \frac{1}{2}\left(\frac{p}{mc}\right)^2\right).$$