Statistical Mechanics II

Jiansheng Wu

Lecture 1

Outline

- Syllabus
- Review of thermodynamics
- What is statistical mechanics?
- Maximum entropy principle

Syllabus: Instructor

Research Field

Superconductivity
and Strongly Correlated System

Disordered System
and Amorphous Solid

Topological Phase of Matter
and Its Application in Spintronics

Superconducting Qubits
and Quantum Simulation

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Jiansheng Wu
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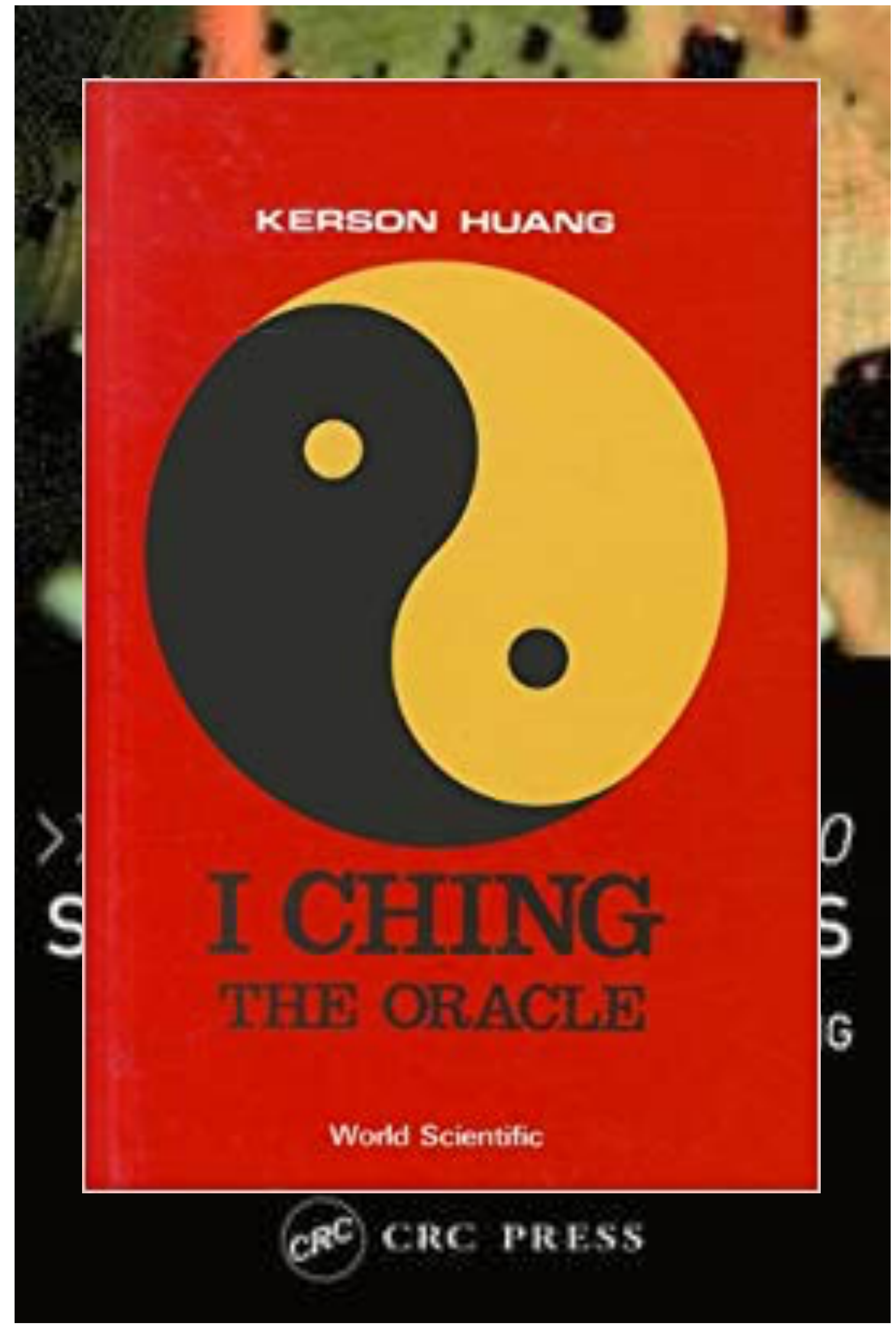
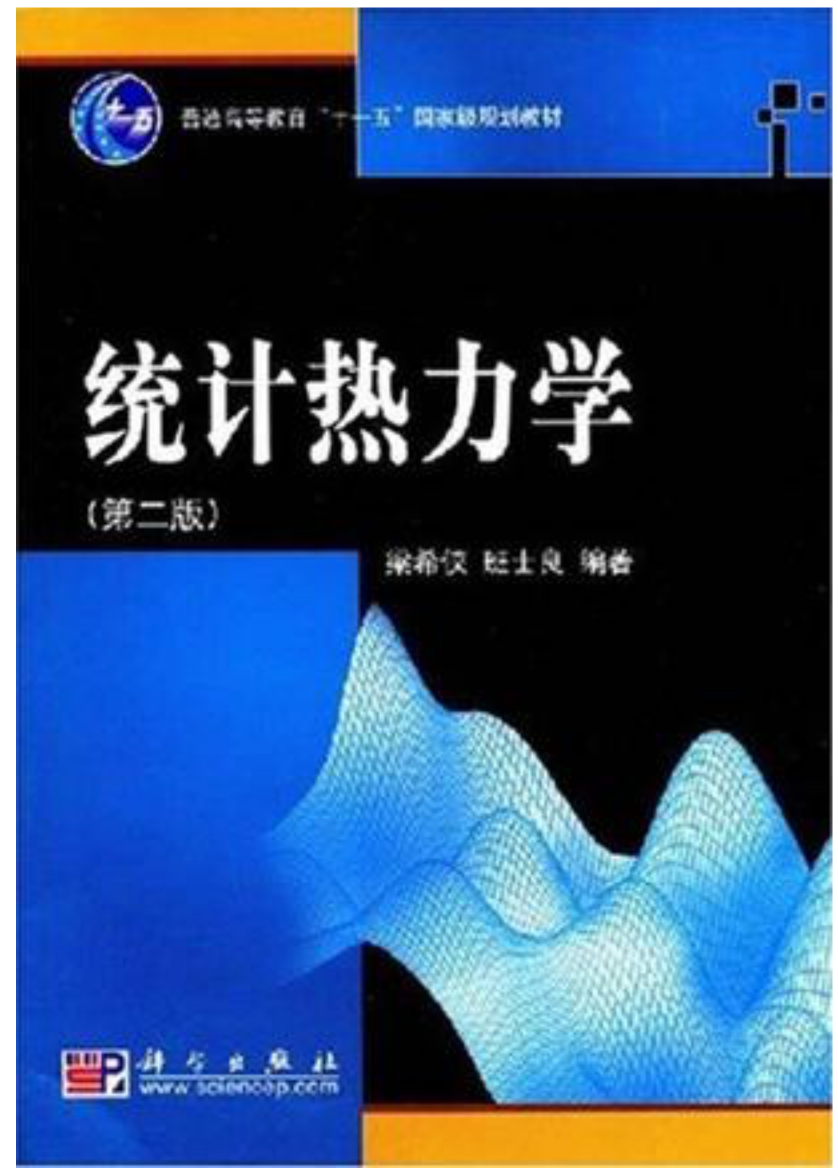
Syllabus: Textbooks

Kerson Huang
（黄克逊）



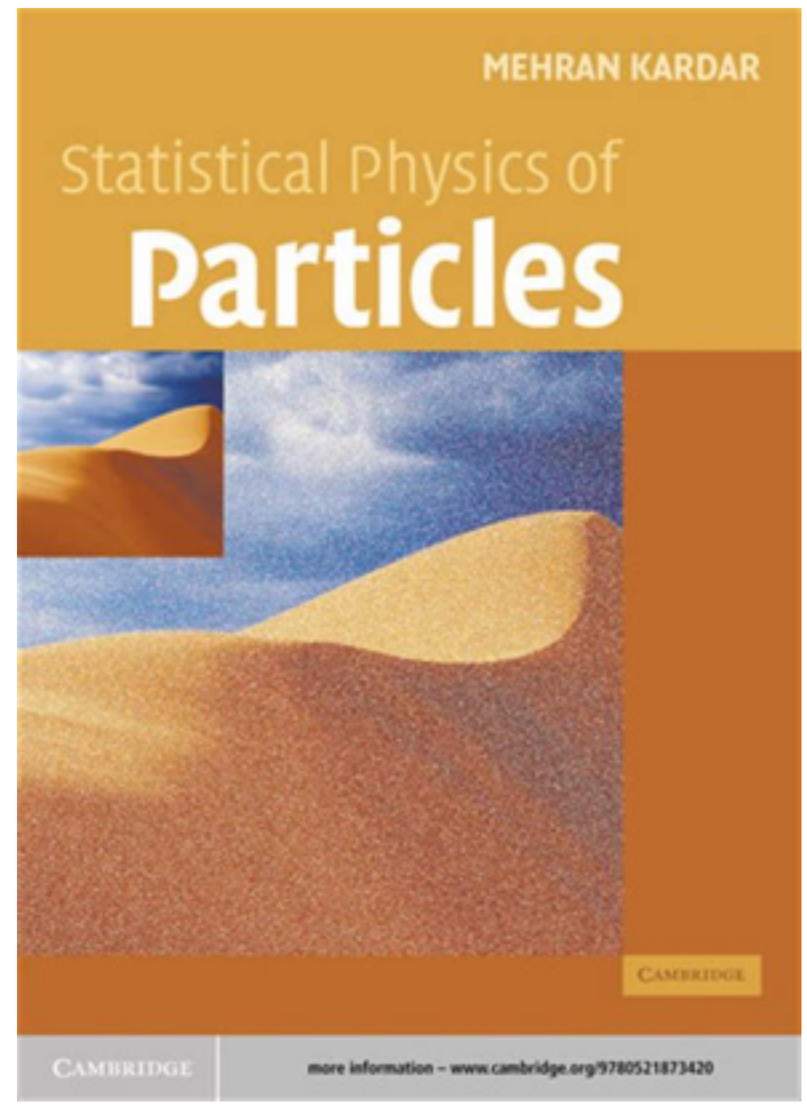
Syllabus: Textbooks

梁希侠



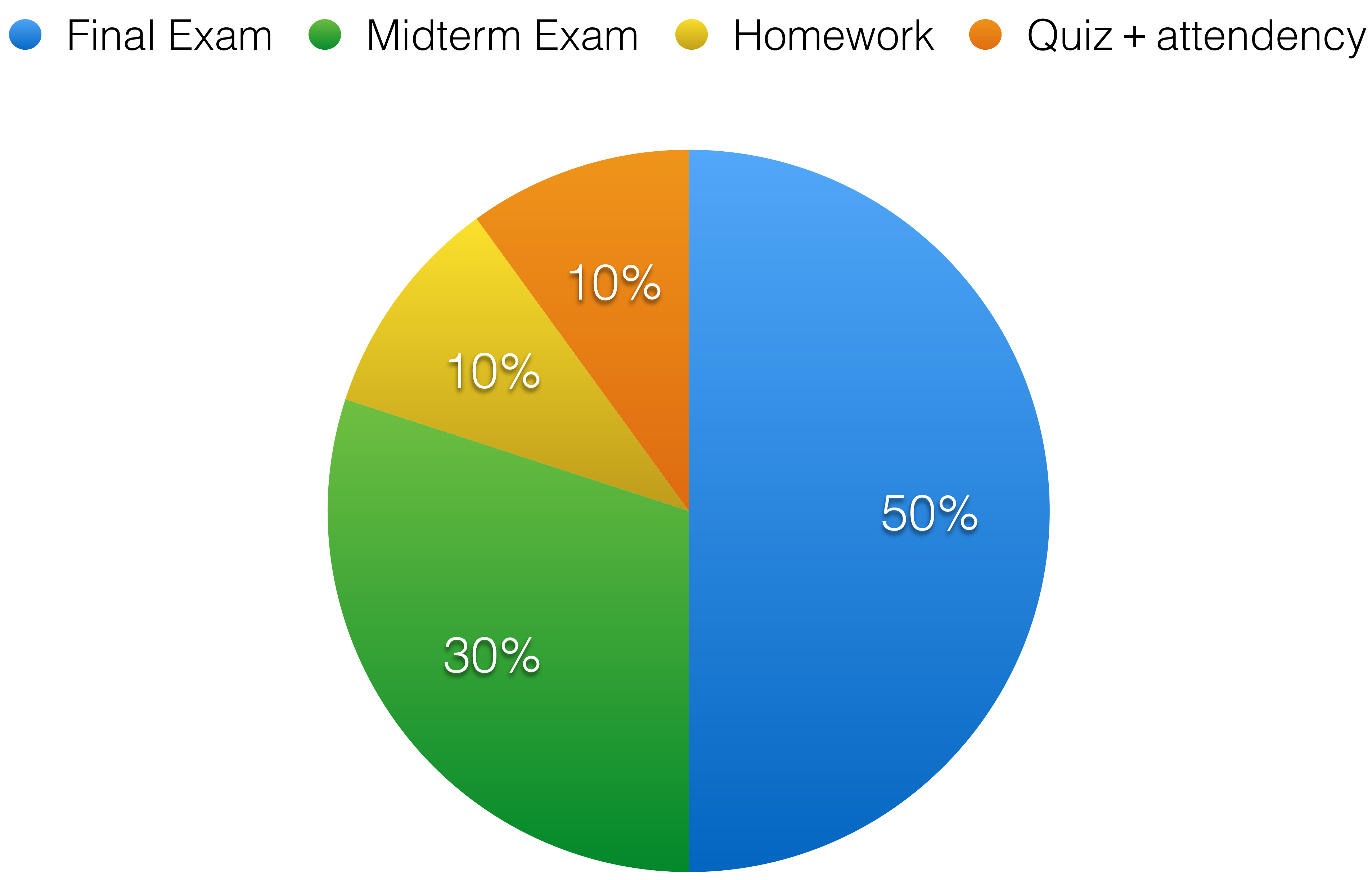
Syllabus: Textbooks

林宗涵



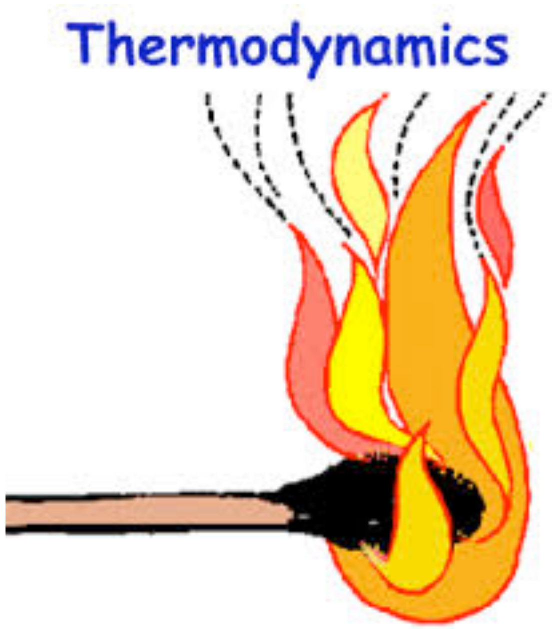
Mehran Kardar

Syllabus： Scores



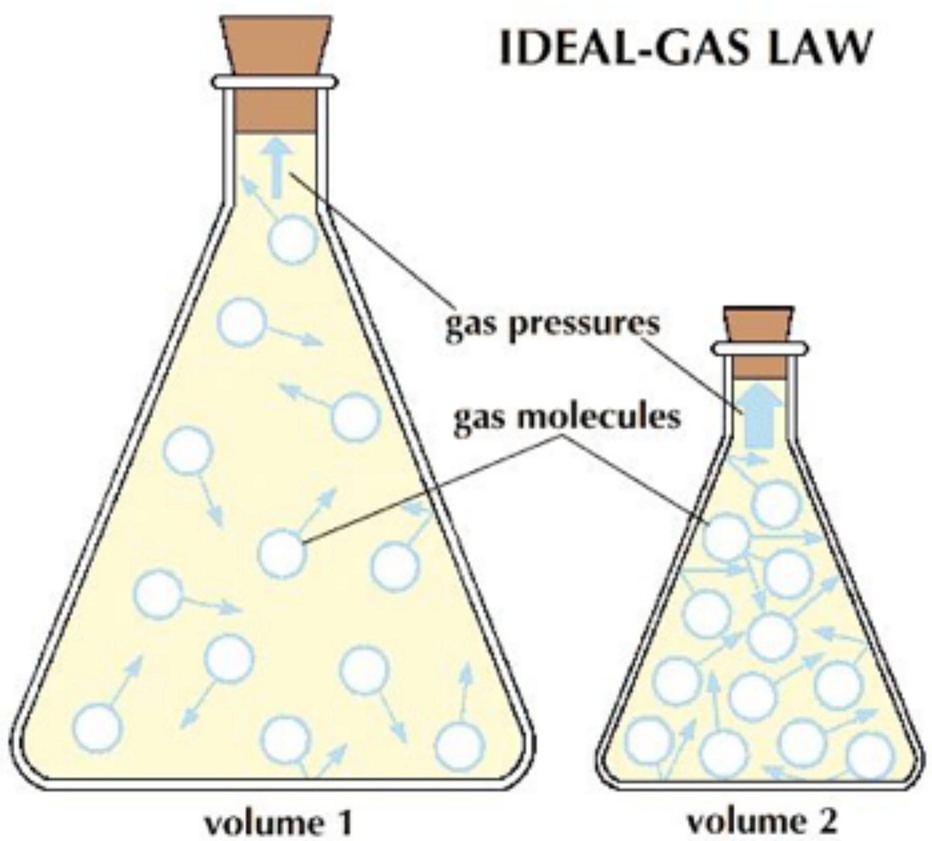
Review： what is Thermodynamics？

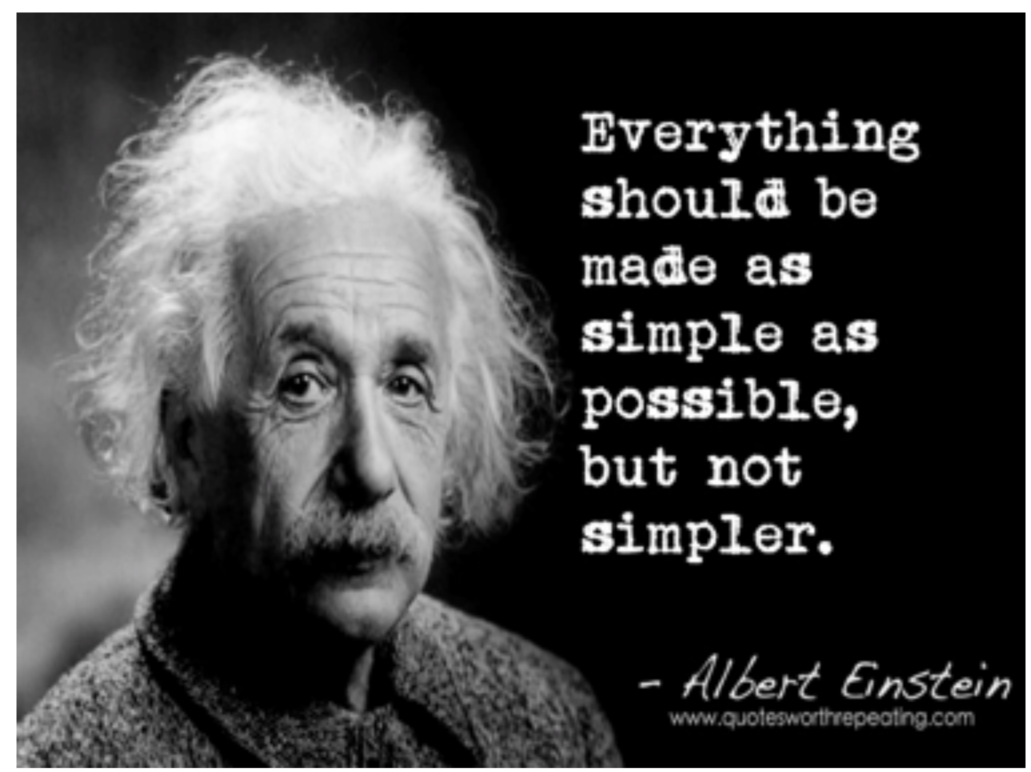
- Thermodynamics is a phenomenological description of properties of macroscopic systems in thermal equilibrium.



How does it work?

1) Idealize the systems: (simplify)

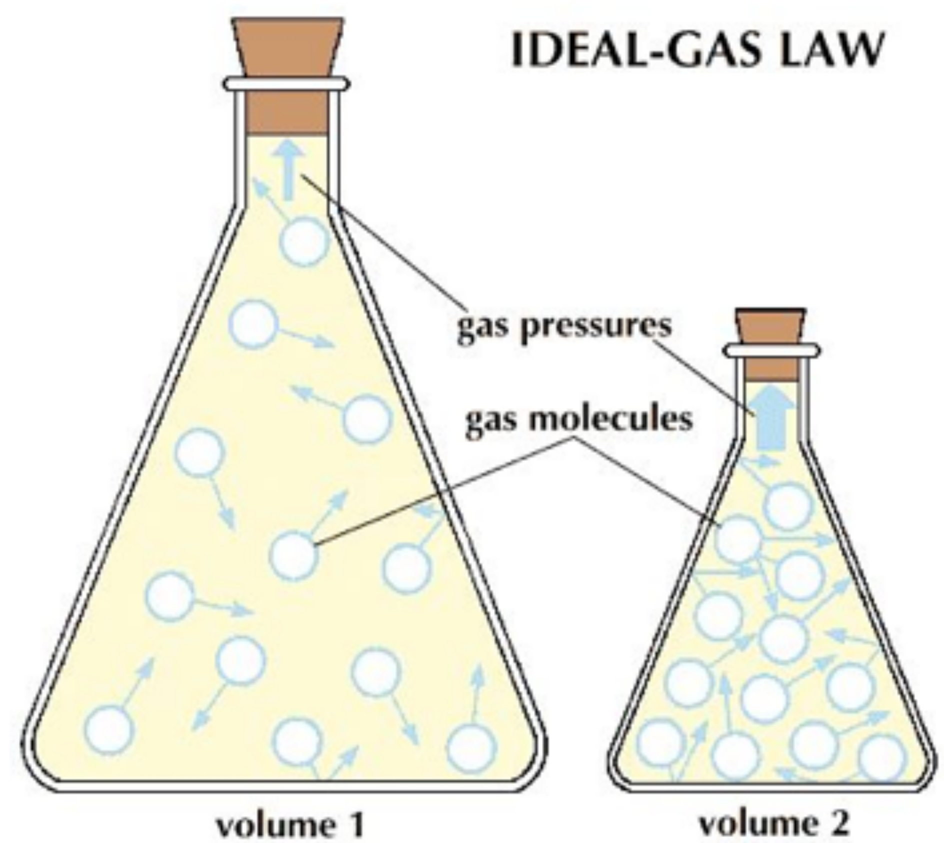




How does it work?

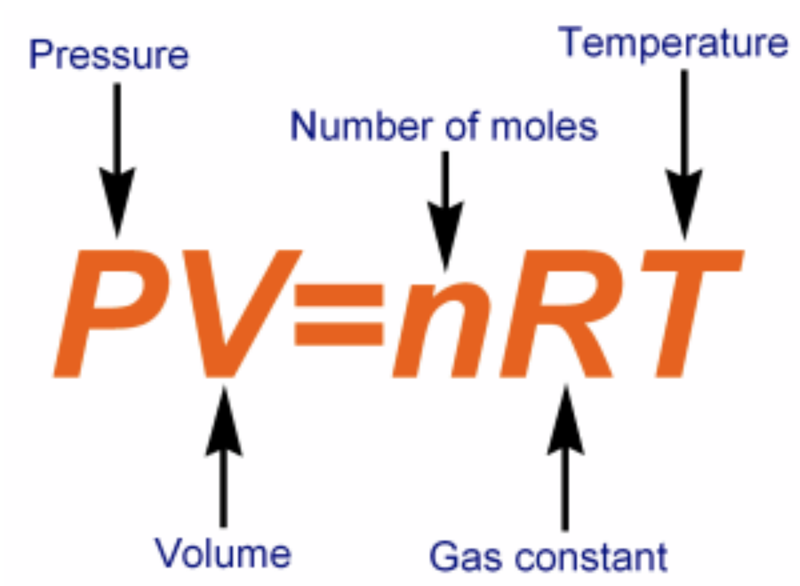
2) State functions: (describe the system, like coordinate of particles)

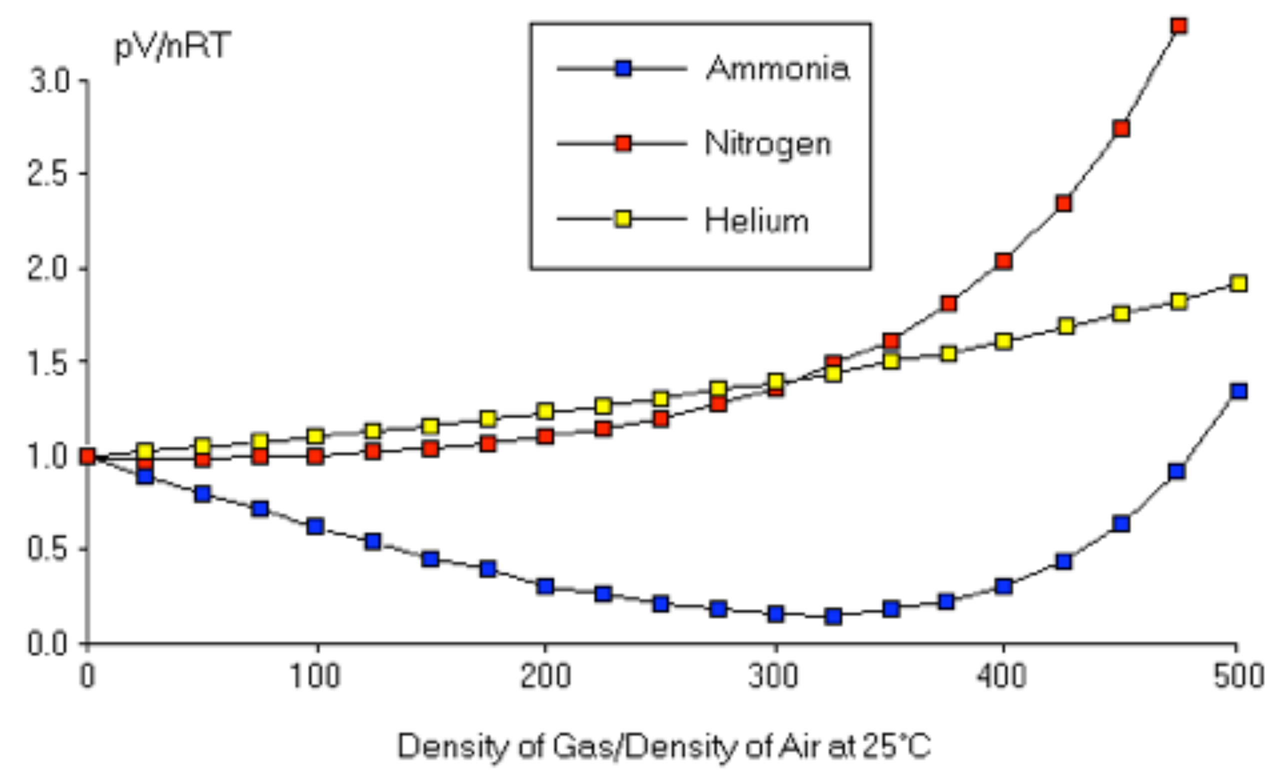
P= pressure
V= volume
n= number of moles
T= temperature
R= the constant



How does it work?

3) Equation of states: (from empirical observations)





4 laws of thermodynamics

1-st law: Energy conservation

2-nd law: Entropy (approaching to equ.)

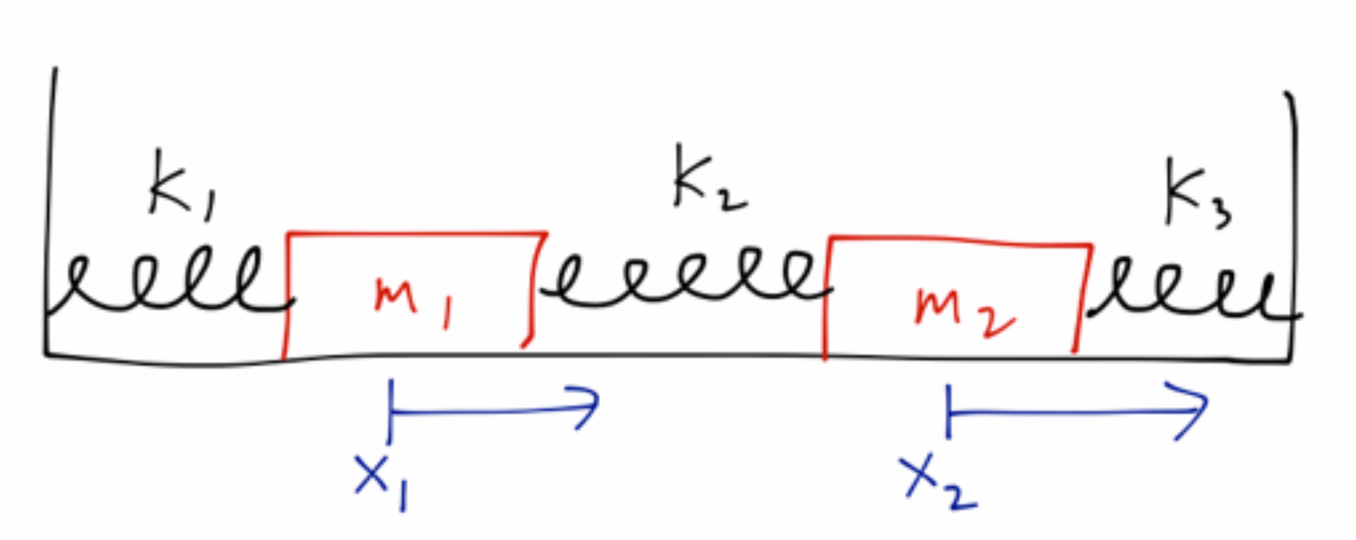
3-nd law: Entropy at zero T is zero

$$\mathrm{d}E = \text{đ}Q + \text{đ}W = T\,\mathrm{d}S + \sum_i J_i\,\mathrm{d}x_i\,.$$

0-th law: Equilibrium

Thermal Equilibrium

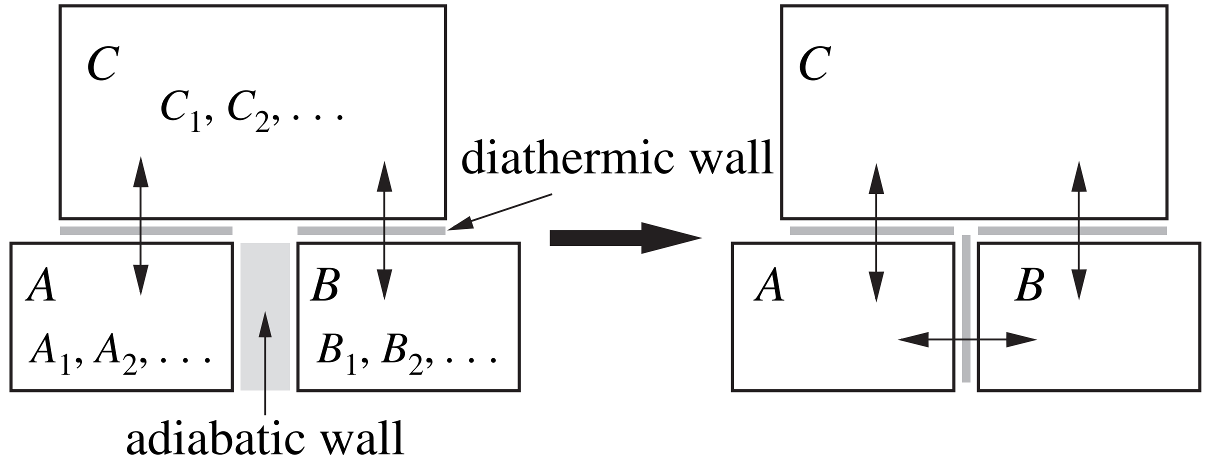
- Mechanical equilibrium:



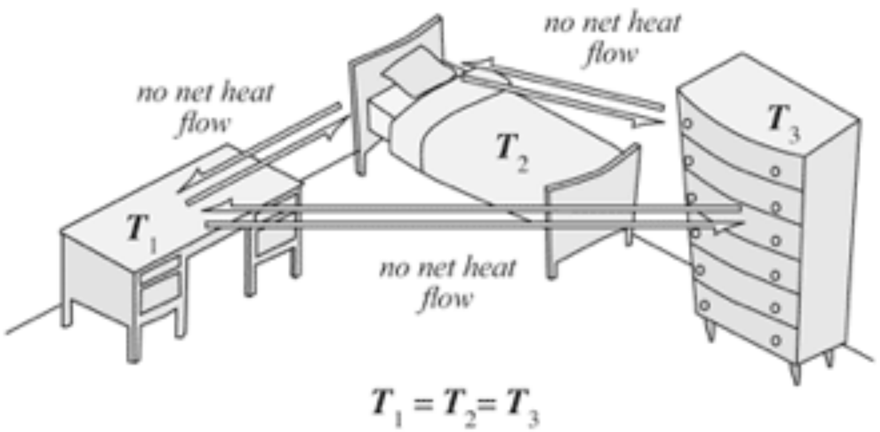
- Thermal equilibrium: A is in thermal equilibrium with B if A is in thermal contact (can exchange heat) with B and no thermodynamics variables of either system are changing.

The 0-th law

- If two systems, A and B, are seperately in equilibrium with a third system C, then they are also in equilibrium with one another
- This defines "temperature" (Systems in equilibrium share



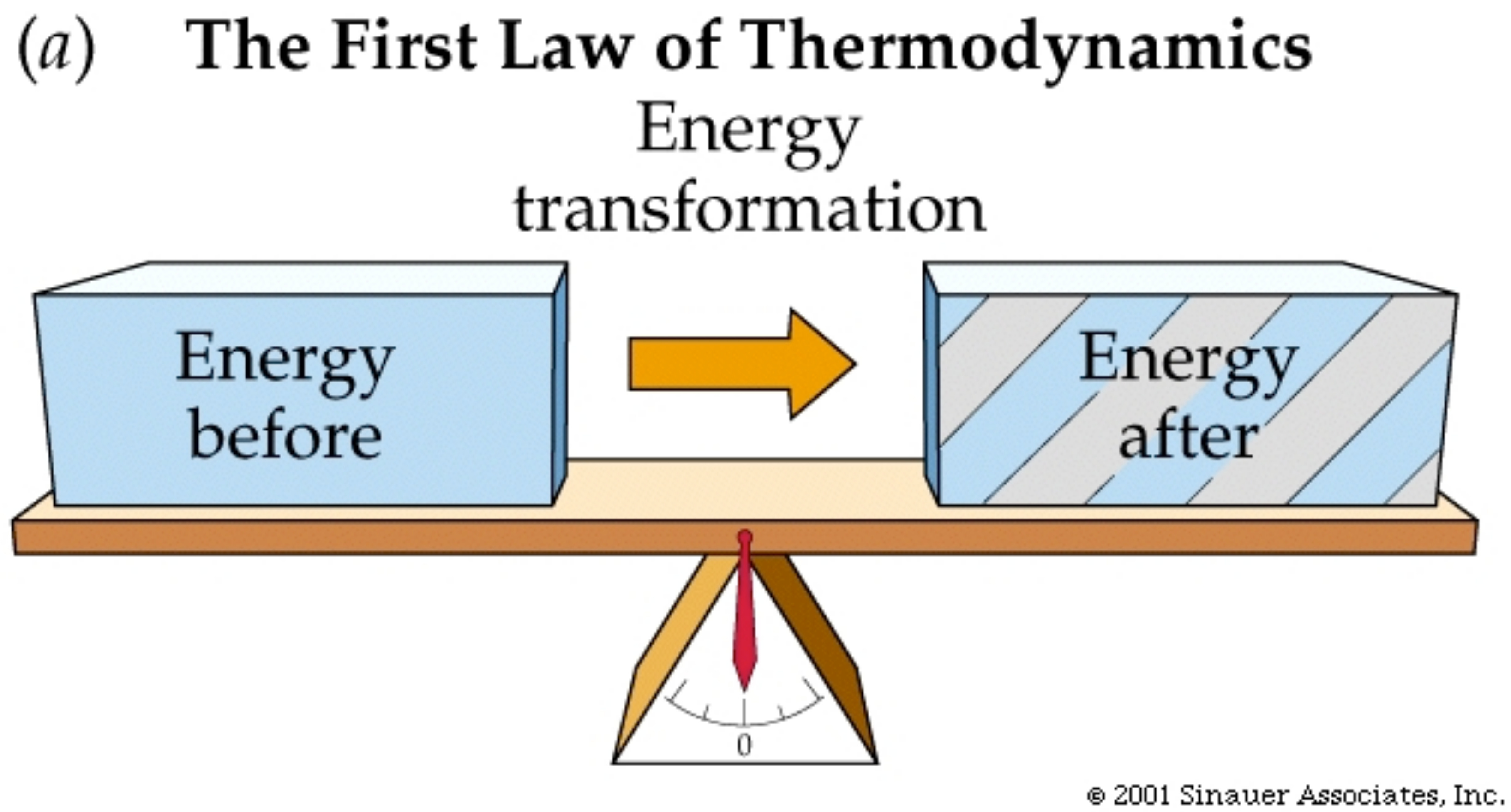
Equilirium is transitive!



Systems at the same temperature are in thermal equilibrium.

The 1st law

$$\mathrm{d}E = đQ + đW$$

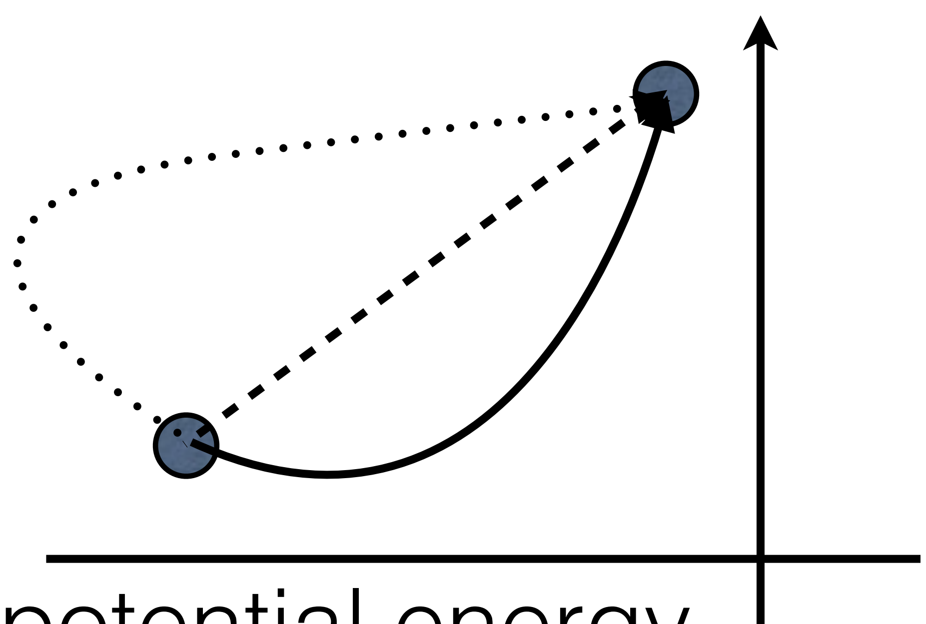


Adiabatically isolated system

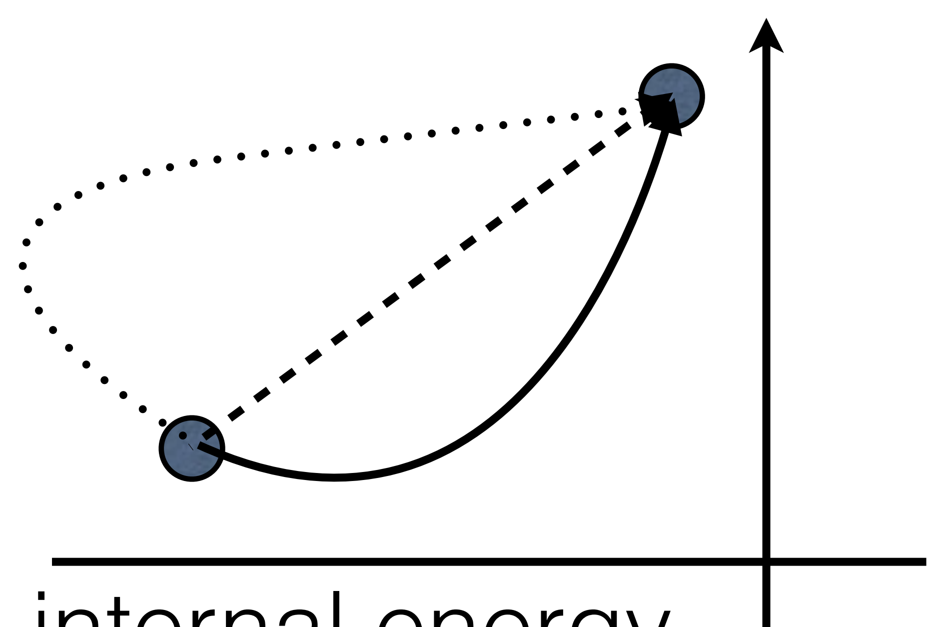
- For a adiabatically isolated system, the amount of work required to change the state depends only on the initial and finally state (Internal energy is a function of state).

$$\Delta W = E(\mathbf{X_f}) - E(\mathbf{X_i})$$

$$\Delta U = mg\int_i^f dl = mg(h_f - h_i)$$



potential energy



internal energy

Work

$$đW = \sum_i J_i \mathrm{d}x_i .$$

Table 1.1 *Generalized forces and displacements*

System	Force		Displacement	
Wire	tension	F	length	L
Film	surface tension	$\mathcal{S}$	area	A
Fluid	pressure	$-P$	volume	V
Magnet	magnetic field	H	magnetization	M
Dielectric	electric field	E	polarization	P
Chemical reaction	chemical potential	μ	particle number	N

Noneadiabatically isolated system

- For a noneadiabatically isolated system, the amount of work is not equal to the change of internal energy. The difference is defined as "heat"(a special kind of energy).

$$đQ = \mathrm{d}E - đW$$

The 1st law is about energy conservation and the energy transformation between work and heat

Entropy

$$đQ = T\,\mathrm{d}S$$

generalized force

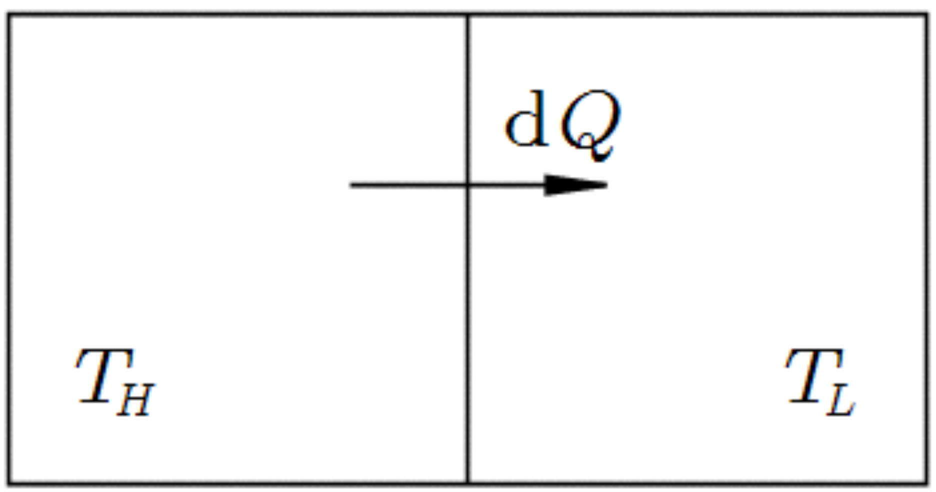
generalized displacement

This define a new function of state, entropy

The 2nd law and arrow of time

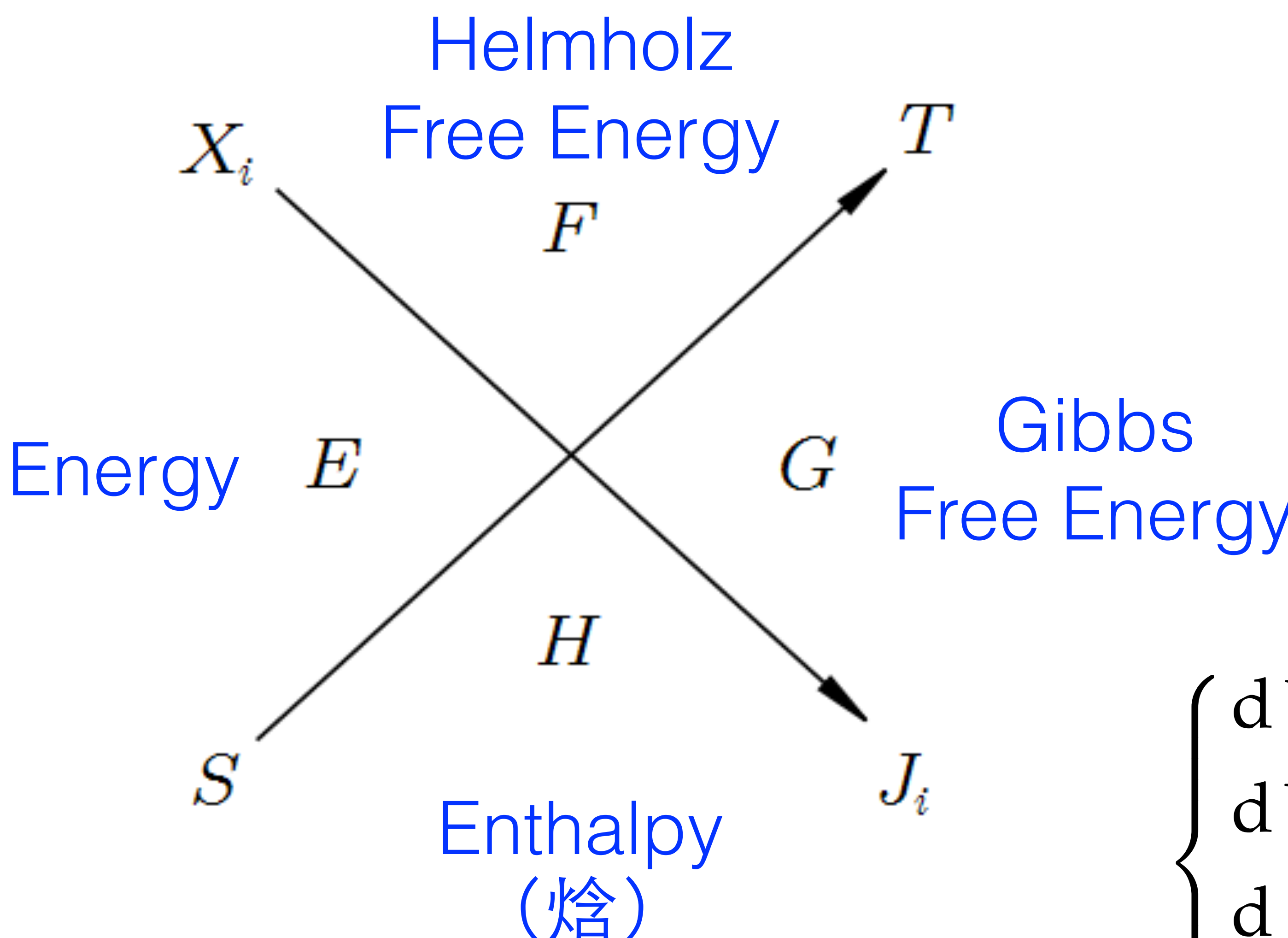
- Consider adiabatically isolating a number of subsystems, each initially separately in equilibrium. As they come to a state of joint equilibrium, $dQ=0$, $dS>0$.
- Thus an adiabatic system attains a maximum value ($dS=0$) of entropy in equilibrium since spontaneous internal change can only increase S ($dS>0$).
- The direction of increasing entropy point out the arrow of time.

Proof： heat transfer from heater to cooler object



$$
\begin{aligned}
dS_{ToT} &= dS_L + dS_R = -\frac{dQ}{T_H} + \frac{dQ}{T_L} \\
&= dQ\left(-\frac{1}{T_H} + \frac{1}{T_L}\right) \geqslant 0
\end{aligned}
$$

Maxwell Relation



$$F = E - TS$$

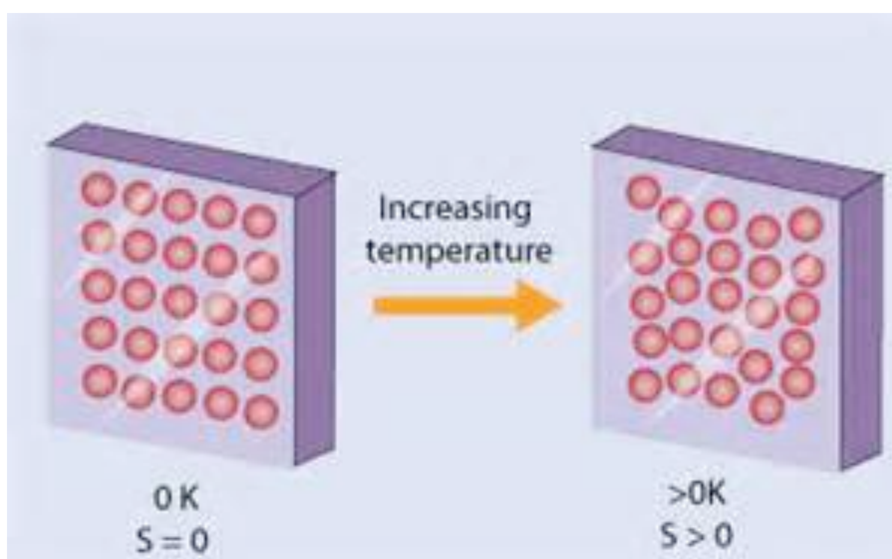
$$H = E - pV = E + J\,x$$

$$G = E - pV - TS$$
$$= E + J\,x - TS$$

$$\begin{cases} dE &= J_i dx_i + TdS \\ dF &= J_i dx_i - SdT \\ dG &= -SdT - x_i dJ_i \\ dH &= -x_i dJ_i + TdS \end{cases}$$

The 3rd law

- The entropy of all systems at zero absolute temperature is a universal constant that can be taken to be zero.
- The "referencing point" of entropy



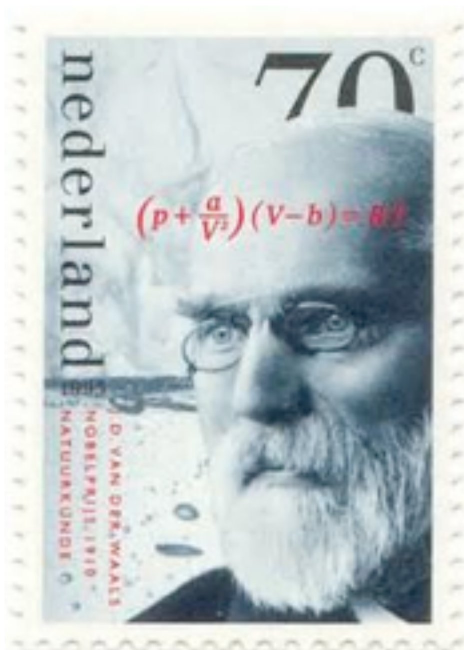
$$\Delta S = \int_i^f \frac{dQ}{T}$$

Summary of 4 laws of thermodynamics

- 0th law: Equilibrium is transitive (Define temperature)
- 1st law: Energy is conserved and can transfer between work and heat (Define heat)
- 2nd/3rd law: Transfer between work and heat has some constraint (Define entropy)

$$dE - đW = đQ = TdS$$

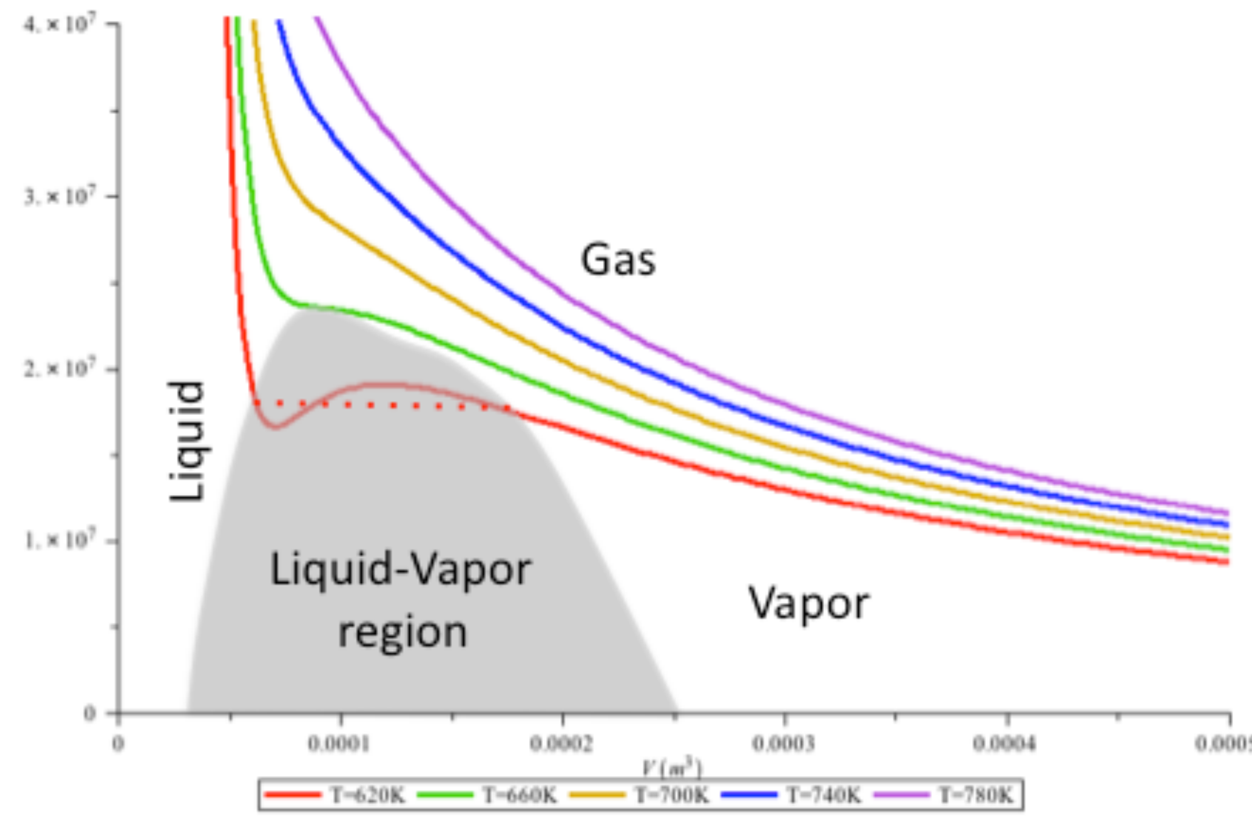
Thermal system 1:
Van der Waals gas



$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT$$

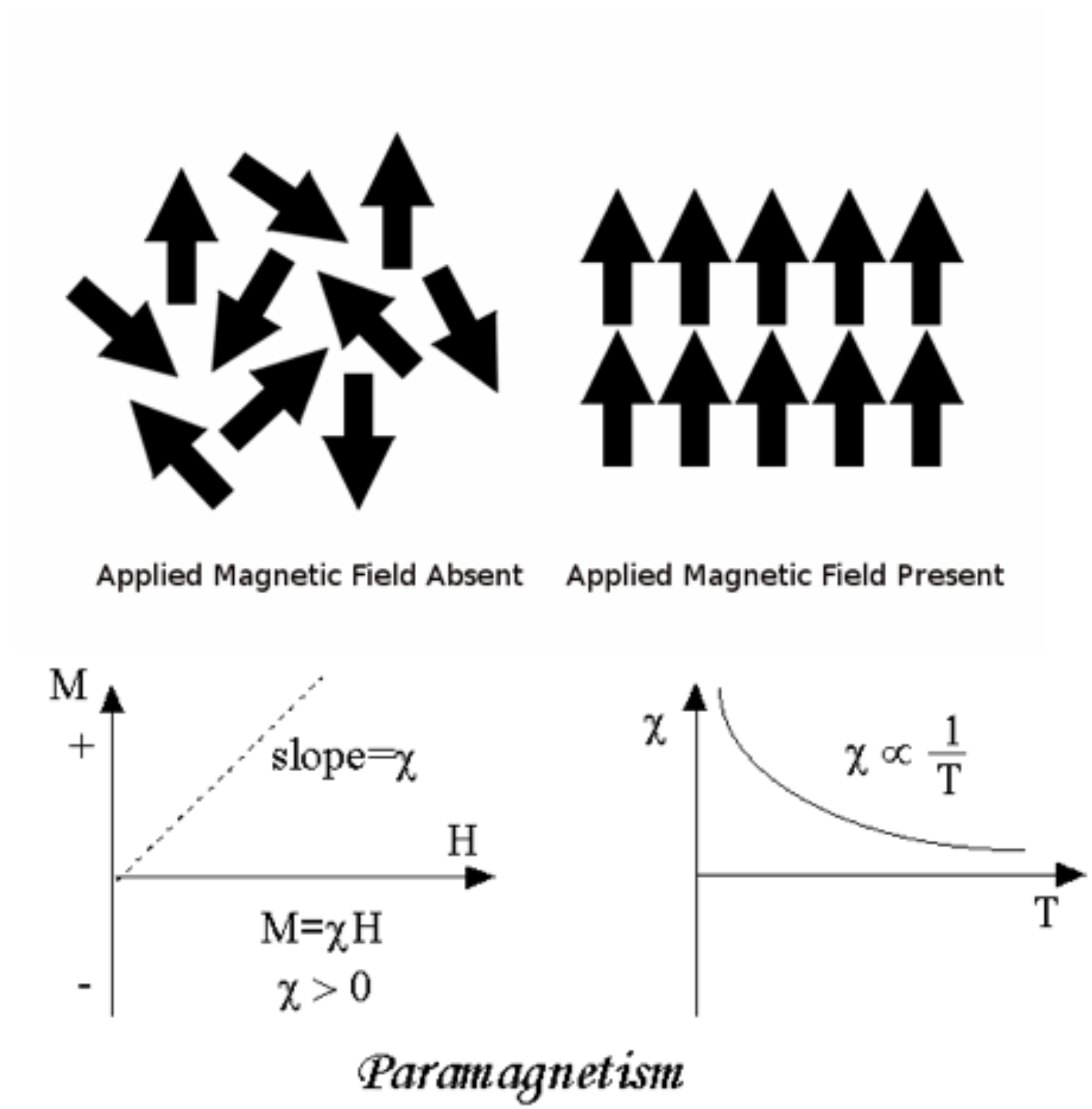
pressure correction term

volume correction term



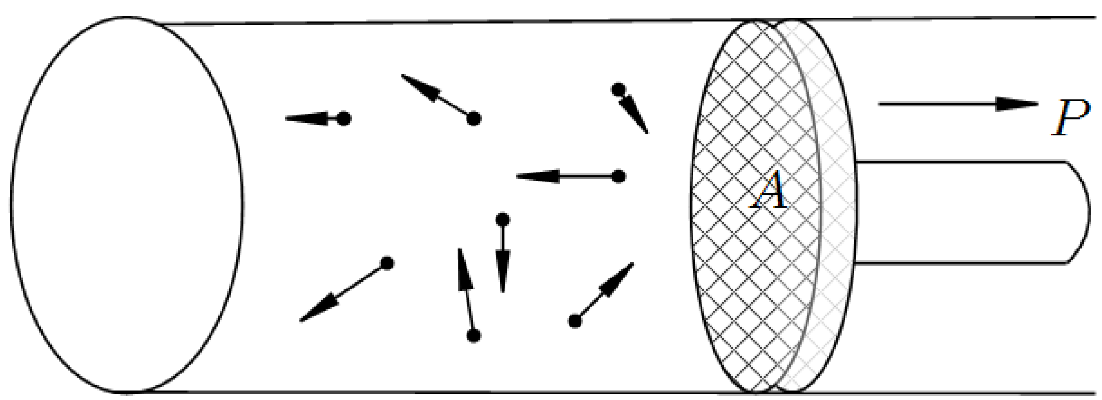
Thermal system 2: Curie's paramaget

- Paramagnetism is a form of magnetism whereby certain materials are attracted by an externally applied magnetic field, and form internal, induced magnetic fields in the direction of the



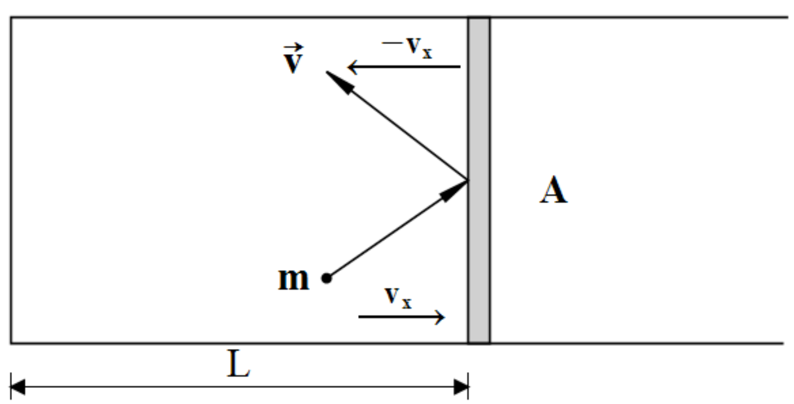
What is statistical mechanics?

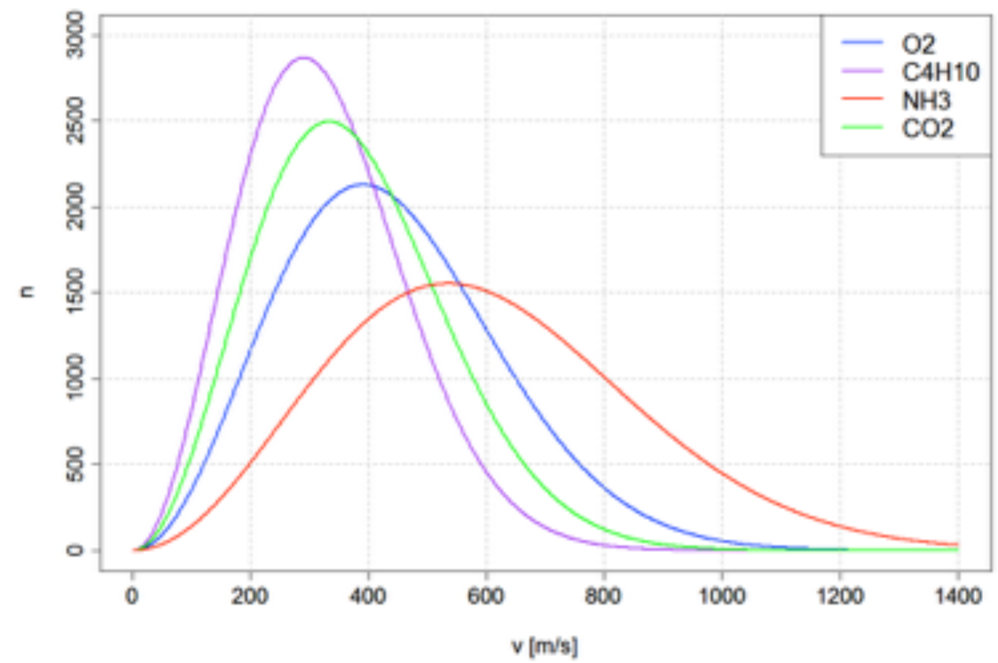
An example in case：Ideal gas



Macroscopic Properties	Analog of mechanical system
P: Presure V: Volume T: Temperature N: Particle Number	like coordinate of a particle
Equation of State: $PV = Nk_BT$	like equation of motion

What is statistical mechanics?





$$
\begin{aligned}
P &\overset{\text{def}}{=} \frac{F}{A} = \frac{\overline{\Delta p/\Delta t N}}{A} \\
&= \frac{1}{A}\left(\frac{\overline{2mv_x}}{2L/v_x}\right) N \qquad * \\
&= \frac{1}{A}\frac{\overline{2mv_x}}{L} N = \frac{N}{V} m\overline{v_x^2} = \frac{N}{V}\frac{1}{3} m\overline{v^2}
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{P}(v) &= \sqrt{\left(\frac{m}{2\pi k_B T}\right)^3} 4\pi v^2 e^{-\frac{mv^2}{2k_B T}} \\
&= \prod_{i=1}^{3} \sqrt{\frac{m}{2\pi k_B T}} e^{-\frac{mv_i^2}{2k_B T}}
\end{aligned}
$$

$$
\begin{aligned}
\langle m v_x^2 \rangle &= \frac{m}{2} \int \mathbf{P}(v_x)\, dv_x = \frac{1}{2} 2 k_B T = k_B T \\
\frac{1}{2}\langle m v^2 \rangle &= \frac{m}{2} \int v^2 P(v)\, dv = \frac{3}{2} k_B T \\
\langle m v^2 \rangle &= 3 k_B T
\end{aligned}
$$

$$
\begin{aligned}
P &= \frac{N}{V}\frac{1}{3} m\overline{v^2} = \frac{N}{V}\frac{1}{3}(3k_B T) = \frac{N k_B T}{V} \\
&\Longrightarrow PV = N k_B T
\end{aligned}
$$

What is statistical mechanics?

$$\boxed{\begin{array}{l}\vec{v}\text{ of each individual particles}\\ \mathrm{P}\left(v\right)\text{ distribution}\end{array}} \overset{SM}{\Longrightarrow} \boxed{\begin{array}{l}\text{Eq. of State}\\ \text{macroscopic properties}\end{array}}$$

Statistical Mechanics is discipline studying many-particle (or more generally, many-agents) system.

Its purpose is to deduct the macroscopic thermodynamic properties of the systems from their microscopic structure.

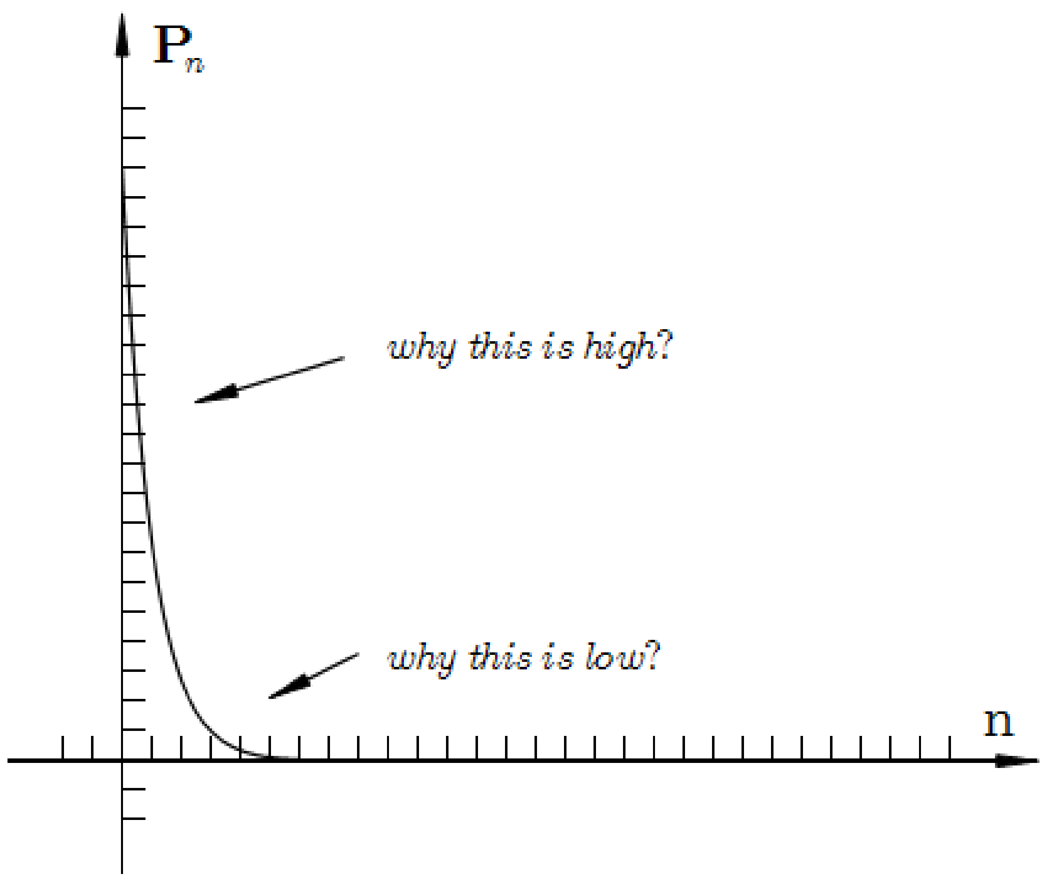
How distribution emerge?

A number game:
1) Write down a table in your paper

1	3
2	4
3	
4	
5	
...	
19	
20	

2) Play a game with another student in class
(a) You two play the SSC game, the person who win the game get one point, the other people lose one point only if both of your points are positive or zero. Otherwise, keep the same points.
(b) If you two play even, don't change you points.
Each person has to play with different people at each time. Stop when you play 19 times.

Distribution



$$\overline{P}_n = N_0 e^{-\beta n}$$

Why? A simple explanation

$n \longrightarrow n+1$ the probability to win 1 point is $\frac{1}{2}$

$n \longrightarrow n+2$ the probability to win 2 points $\left(\frac{1}{2}\right)^2$

....

$n \longrightarrow n+s$ the probability to win s points is $\left(\frac{1}{2}\right)^s$

$$= e^{\ln\left(\frac{1}{2}\right)^s} = e^{s\ln\frac{1}{2}} = e^{-s\ln 2}$$

Why? A formal explanation

$$\begin{cases} \sum_n P_n & = N_s \\ \sum_n n P_n & = N_p \end{cases}$$

"that how do you put N_p balls into N_s boxes."

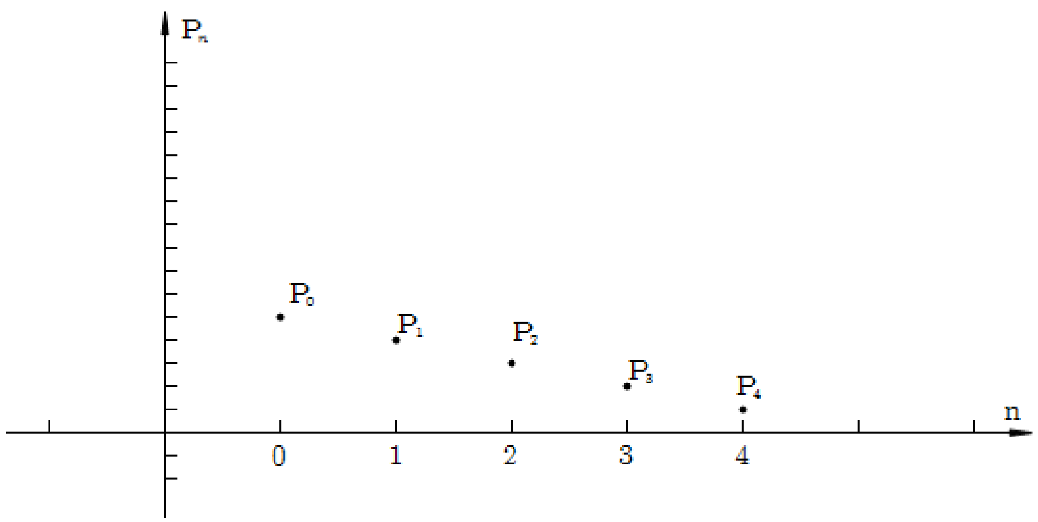
$$N_p = 4, \qquad N_s = 3$$

marcrostates	0	1	2	3	4	number of microstates	probability
0+0+4	2	0	0	0	1	$\frac{3!}{2!1!} = 3$	20%
0+1+3	1	1	0	1	0	$\frac{3!}{1!1!1!} = 6$	40%
0+2+2	1	0	2	0	0	$\frac{3!}{1!2!} = 3$	20%
1+1+2	0	2	1	0	0	$\frac{3!}{2!1!} = 3$	20%

distribution

highest probability

General case



$$\Omega = \frac{N_p!}{P_1!P_2!\cdots P_{N_s}}$$

$$\begin{aligned} S &= \ln \Omega \\ &= \ln \frac{N_p!}{P_1!P_2!\cdots P_{N_s}} \end{aligned}$$

maximize S s.t. $\begin{cases} \sum_n P_n & = N_s \\ \sum_n n P_n & = N_p \end{cases}$

Lagrange multiplier

$$\delta \left[\ln \Omega \{P_n\} - \alpha \sum_n P_n - \beta \sum_n n P_n \right] = 0$$

Exponential distribution

$$\ln \Omega\{P_n\} = \ln N_p! - \sum_n \ln P_n!$$
$$= \ln N_p! - \sum_n P_n \ln P_n + \sum_n P_n$$

Stirling formula

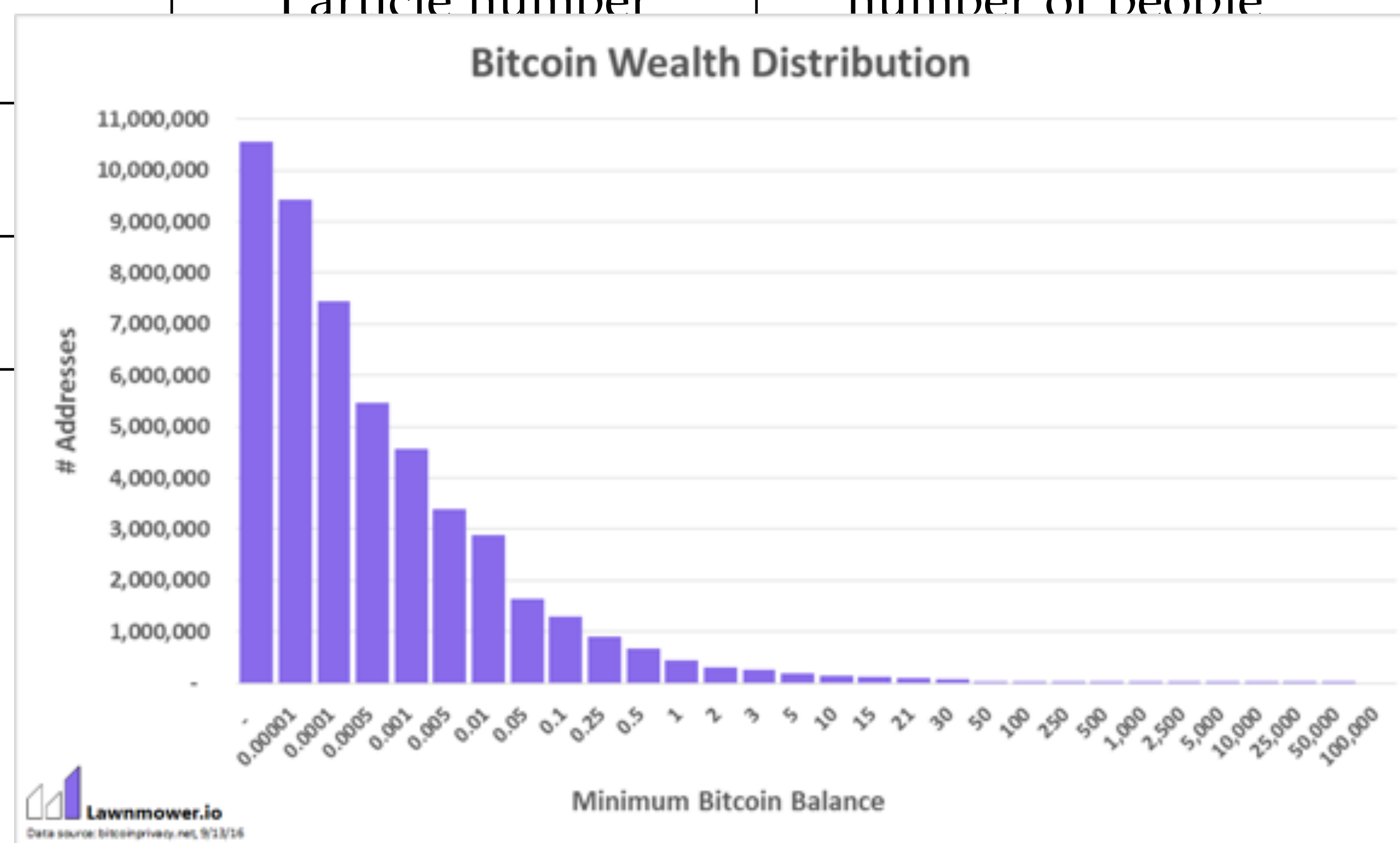
$$\ln P_n! = P_n \ln P_n - P_n$$

$$0 = \delta \sum_n \left[-P_n \ln P_n + P_n - \alpha P_n - \beta n P_n\right]$$
$$= \sum_n \left[-\ln P_n - P_n \frac{\delta \ln P_n}{\delta P_n} + 1 - \alpha - \beta n\right] \delta P_n$$
$$= \sum_n \left[-\ln P_n - \alpha - \beta n\right] \delta P_n$$

$$P_n = e^{-\alpha - \beta n} = N_0 e^{-\beta n}$$

Exponential distribution

Game	Ideal gas	Distribution of wealth
Students	Particles	People
Points	Energy	Wealth
Playing a game between two students	Collisions of particles	Transfer of wealth
Students number is fixed	Particle number	number of people
Total # of points are		
Most probable configuration		

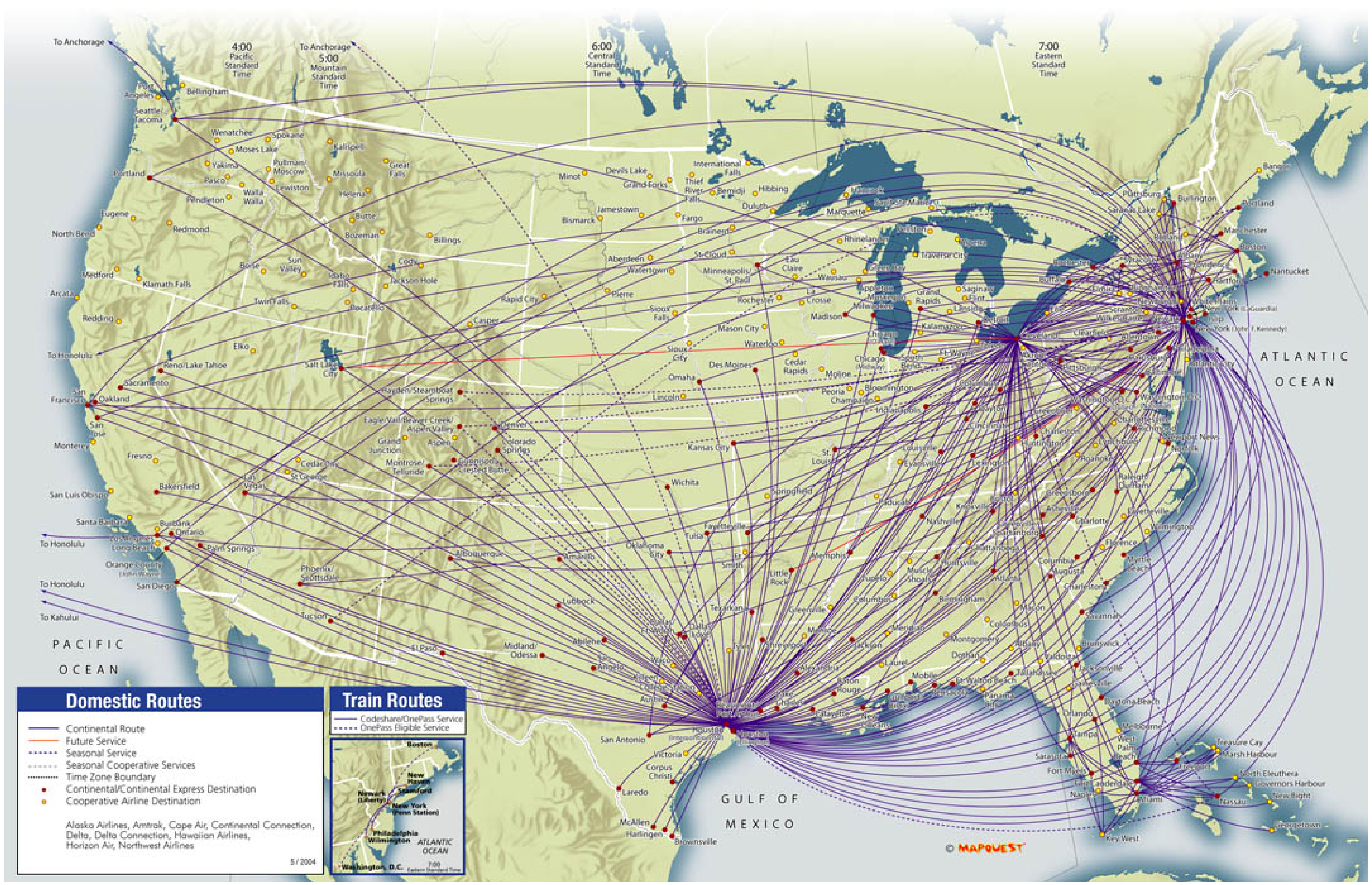


What is statistical mechanics?

$$\boxed{\begin{array}{c}\text{Macroscopic}\\ \text{properties}\\ \text{(Eq. of States)}\end{array}} \xleftarrow{SM} \boxed{\begin{array}{c}\text{Microscopic}\\ \text{Structure}\\ \text{(Distribution)}\end{array}} \longleftarrow \boxed{\begin{array}{c}\text{Most probable distribution}\\ \text{(biggest number of microstate)}\end{array}}$$

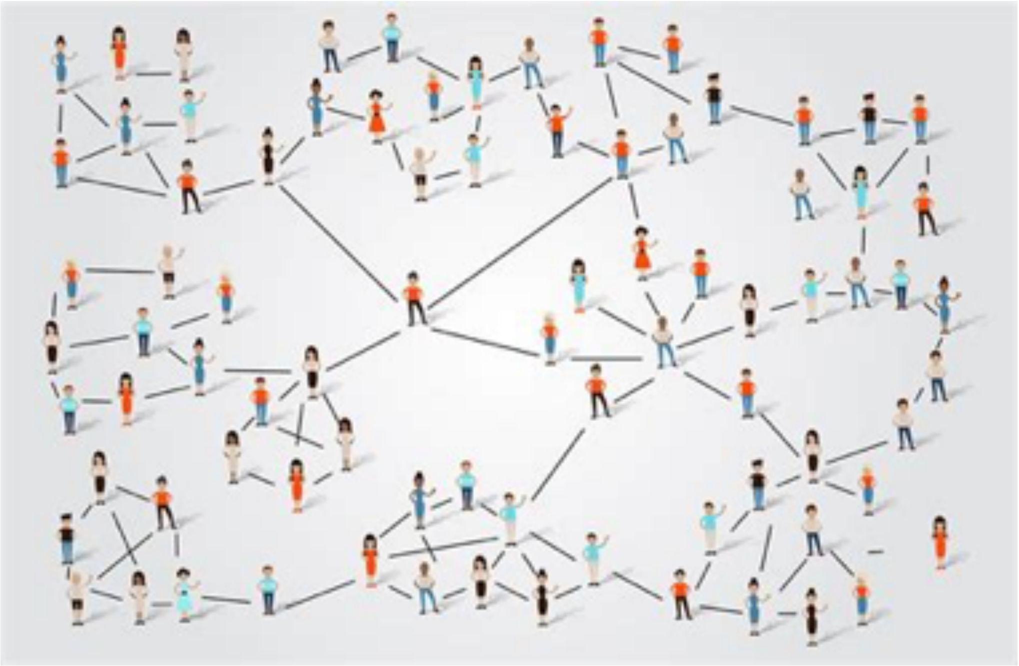
Statistical Mechanics describe the global (macroscopic) properties of a system which consist of many interacting degree of freedom. (particles/ fields/ stocks/ people/ cars. . .). Its purpose is to deduct the macroscopic properties of the systems from their microscopic structure.

Network science

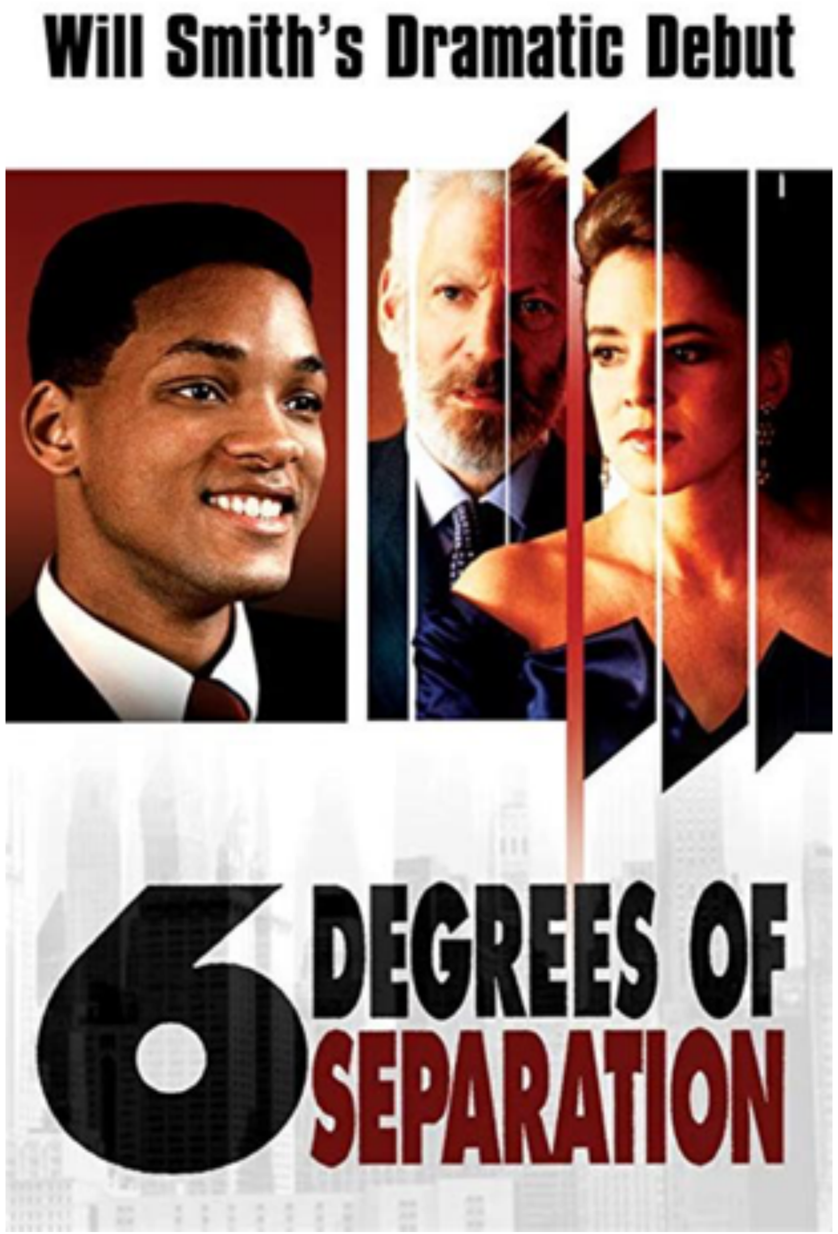


Optimization

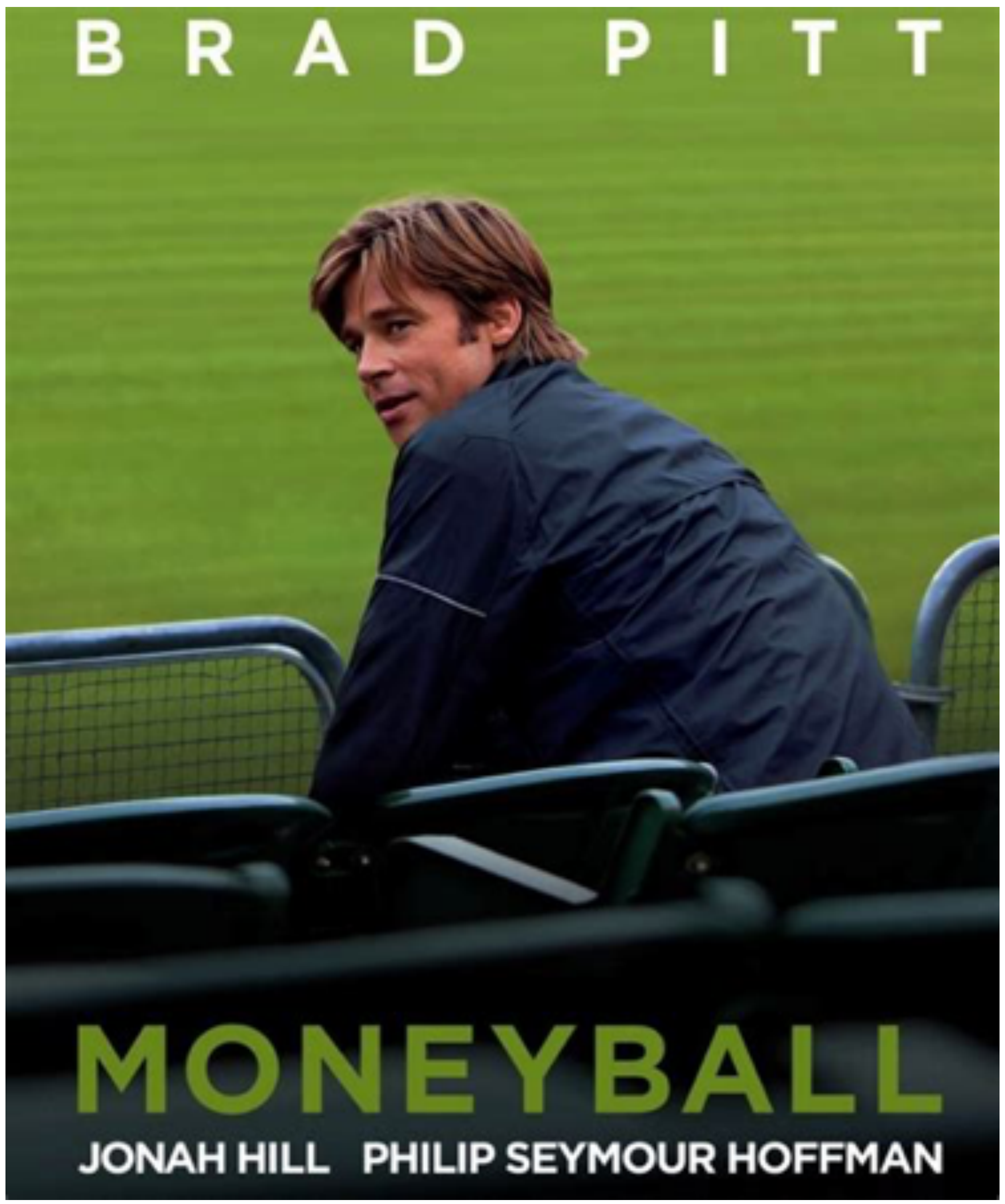
6 degree of separation

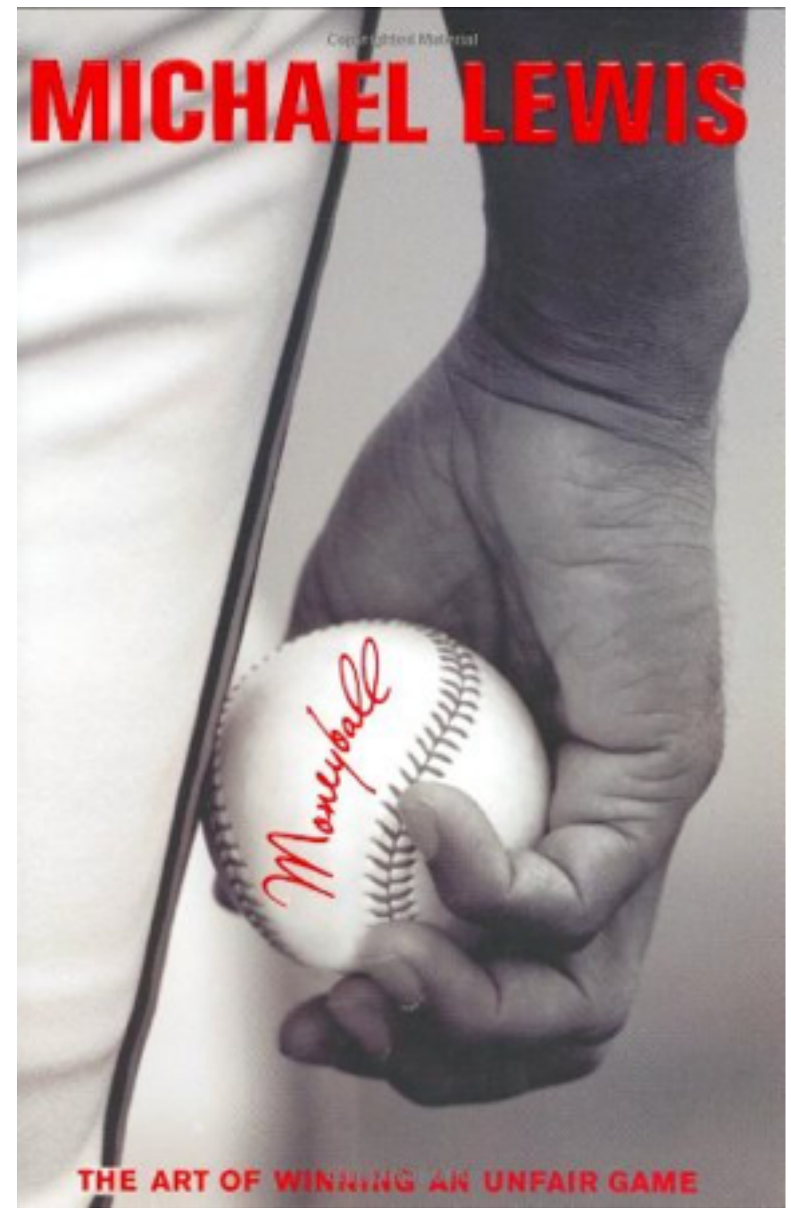


Year	Distance	
2008	5.28	
2011	4.74	
2016	4.57	
Distances as reported in Feb 2016 [38][41]		



Money ball





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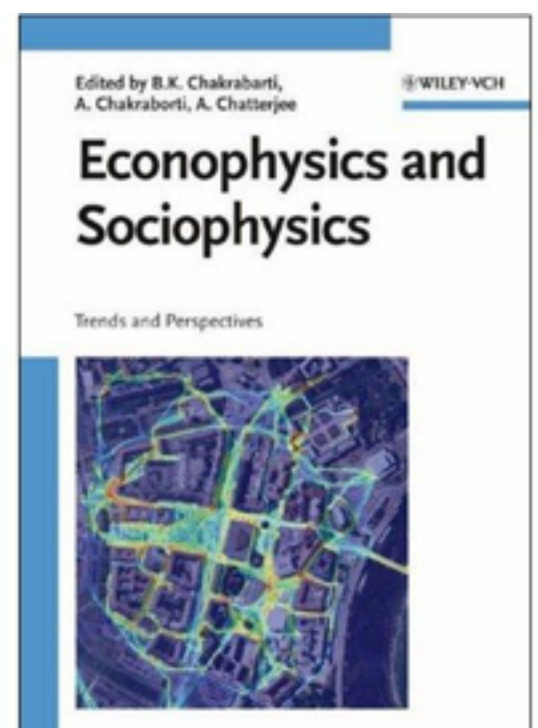
Econphysics and quantitative analyst

Big data analysis in finance and economics
Classical and quantum information
Complex systems
Derivatives pricing
Dynamical and stochastic processes
Econophysics
Financial econometrics
High-frequency trading and its analysis
Incomplete markets
Mathematical finance
Numerical methods for finance and economics
Phase-transition phenomenon
Random systems
Social-phase transition
Statistical mechanics for financial applications
Stochastic process for finance
Systemic and liquidity risks



Structure of knowledge

Phenomena: Stars won't fall down but apple will. —— Tycho

↑

Phenominological theory —— Kelvin

↑

Microscopic model, mechanism —— Newton

↑

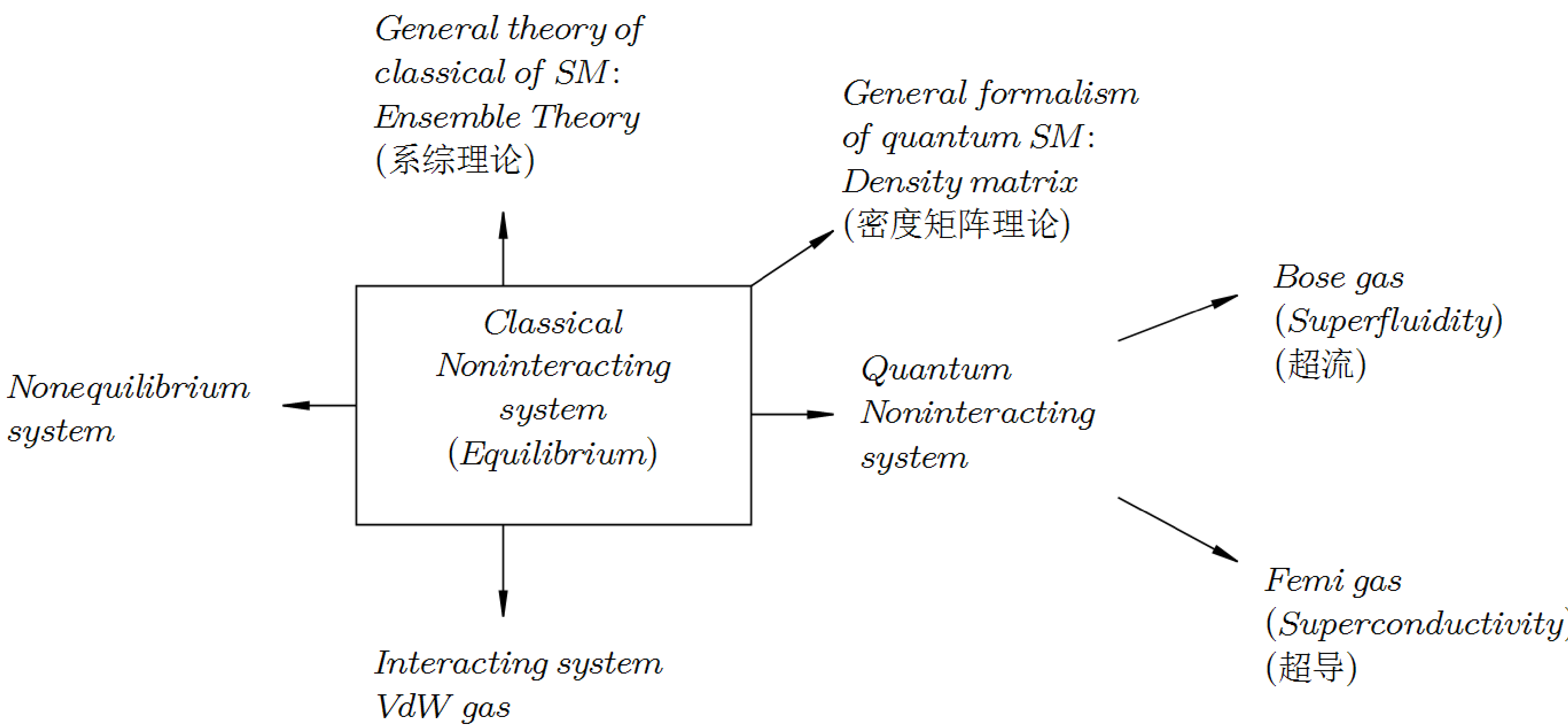
Principle —— Einstein

↑

Philosophy

1. Phenomena	Thermal phenomena
2. Phenomenological theory	↑ Thermodynamics (TD) * P, V, T; State function to represent the state of the system Eq. of state $PV = Nk_BT$
3. Microscopic theory (mechanism)	↑ Statistical Mechanics
4. Principle	↑ Information theory (complexity, entropy)

Roadmap


General theory of
classical of SM:
Ensemble Theory
(系综理论)
General formalism
of quantum SM:
Density matrix
(密度矩阵理论)
Classical
Noninteracting
system
(Equilibrium)
Nonequilibrium
system
Quantum
Noninteracting
system
Bose gas
(Superfluidity)
(超流)
Femi gas
(Superconductivity)
(超导)
Interacting system
VdW gas

Roadmap

<table>
<tr><td>1. Thermodynamics Review</td><td rowspan="2">Preparation knowledge</td></tr>
<tr><td>2.Fundamental knowledge
Probability
Entropy, density of state
(macrostate, microstates)</td></tr>
<tr><td>3. SM of noninteracting system
(Classical & Quantum)</td><td rowspan="6">Macroscopic quantities $\langle O(\Gamma)\rangle$
$\uparrow$
Distribution $P(\Gamma)$
$\uparrow$
Microscopic structure
$H(\Gamma), \Gamma = (\vec{p}_i, \vec{q}_i)$
(Distribution function
and moments)</td></tr>
<tr><td>4. Classical SM (Ensemble Theory)
Microcannonical Ensemble
Cannonical Ensemble
Grand Cannonical Ensemble</td></tr>
<tr><td>5. SM of Interacting System
VdW gas
1st order phase transition</td></tr>
<tr><td>6. Quantum Statistical Mechanics
Why quantum?
General formalism</td></tr>
<tr><td>7. Bosonic gas $\longrightarrow$ Superfluidity</td></tr>
<tr><td>8. Femionic gas $\longrightarrow$ Superconductivity</td></tr>
<tr><td>9. Nonequilibrium System</td><td>$P(\Gamma, t) \longleftarrow$ by time-dependent
differential equations</td></tr>
</table>

Summary

- Review of thermodynamics （4 laws／2 systems／1 Maxwell relation）
- What is statistical mechanics?（Deduce the thermal properties from distribution）
- Maximum entropy principle

Homework 1

PROBLEM 1: Find a the most probable distribution P_n such that,

$$\sum_n P_n = N$$
$$\sum_n nP_n = Nn_a$$
$$\sum_n n^2 P_n = Nn_d^2$$

Here the most probable distribution is defined as the distribution P_n of which the following quantity

$$\begin{aligned} \ln \Omega \{P_n\} &= \ln N_p! - \sum_n \ln P_n! \\ &= \ln N_p! - \sum_n P_n \ln P_n + P_n \end{aligned}$$

is maximized.

PROBLEM 2: For a ideal gas with distribution

$$P(\nu) = \prod_{i=1}^{3} \sqrt{\frac{m}{2\pi k_B T}} e^{-\frac{m(\nu_i - \bar{\nu}_i)^2}{2k_B T}}$$

Please find out the state equation.