

Title: PSI 2019/2020 - Statistical Physics - Lecture 1

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STATISTICAL PHYSICS PRIMER

OUR GOAL: MAKE YOU READY FOR PEDRO'S COURSE

← ENSEMBLES
← TD APPROACH TO PHASE TRANSITIONS
← MICROSCOPIC APPROACH TO PT

1) BASICS OF STATISTICAL PHYSICS

a) FROM QUANTUM TO CLASSICAL

QUANTUM SYSTEMS . • PURE STATE
(MICROSTATE)

$$|\psi\rangle \in \mathcal{H}$$

• MIXED STATE
(MACROSCOPIC STATE)

$$\rho = \sum_{\lambda} p_{\lambda} |\psi_{\lambda}\rangle \langle \psi_{\lambda}|$$

↑
PROBABILITY

TIME EVOLUTION:

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar} [H, \rho]$$

VON NEUMANN EQ.

CHECK. $S = |\psi\rangle\langle\psi|$
 with $\frac{\partial |\psi\rangle}{\partial t} = H|\psi\rangle$ ☺

- $\text{Tr}(\rho) = 1$ ($\sum_{\lambda} p_{\lambda} = 1$)

- EXPECTATION VALUE OF AN OBSERVABLE A

$$a = \text{Tr}(\rho A)$$

- $\text{Tr}(\rho^2) < 1$... PURE
 SOMETHING ELSE ... MIXED

- WHEN ARE WE CLASSICAL?

HEISENBERG

$$\Delta x \Delta p \gg \hbar$$

THERMAL FLUCTUATIONS

$$\frac{(\Delta p)^2}{2m} \approx k_B T, \quad \Delta x = \left(\frac{V}{N} \right)^{1/3}$$

$$\left(\frac{V}{N} \right)^{1/3} \sqrt{2m k_B T} \gg \hbar$$

$$k_B T \gg m^{2/3} \frac{\hbar^2}{2m}$$

$$m = \frac{M}{V}$$

CLASSICAL ?

$$\Delta x \Delta p \gg \hbar$$

THERMAL FLUCTUATIONS

$$k_B T, \Delta x = \left(\frac{V}{N} \right)^{1/3}$$

$$T \gg \hbar$$

$$T \gg m \frac{\hbar^2}{2m}$$

$$n = \frac{N}{V}$$

• IN CLASSICAL PHYSICS

MICROSTATE .. VECTOR IN $6N$ -DIM.

PHASE SPACE $\cdot \Sigma N = \mathbb{R}^{6N}$
 $(\vec{q}_1, \vec{p}_1, \vec{q}_2, \dots, \vec{q}_N, \vec{p}_N)$

• MACROSTATE .. PROBABILITY DISTR.

$$\Omega_N(\vec{q}_1, \dots, \vec{p}_N)$$

= MEASURE

$$\mu = N d\tilde{\gamma}_N$$

$$d\tilde{\gamma}_N = \frac{1}{N! (2\pi\hbar)^{3N}} d^3p_1 d^3q_1 \dots d^3p_N d^3q_N$$

STAT. ENSEMBLE = LARGE # OF BOXES WITH
THE SAME MACROSTATE I FIND CORRESPONDING
MICROSTATE WITH PROBABILITY μ .

$$\langle A \rangle = \int A(p, q) \underbrace{\rho(p, q) d\Gamma_N}_{\text{probability density}}$$

$$\frac{1}{(2\pi\hbar)^{3N}} d^3p_1 d^3q_1 \dots d^3p_N d^3q_N$$

= LARGE # OF BOXES WITH
 MICROSTATE I FIND CORRESPONDING
 E WITH PROBABILITY $\frac{1}{\Omega}$.

DESCRIPTION STAGE	QUANTUM HILBERT SPACE $\mathcal{H}$	CLASSICAL PHASE SPACE Σ_H
MATH	$\text{Tr}(\cdot)$	$\int \cdot d\gamma_H$
STATISTICAL ENSEMBLE	DENSITY MATRIX ρ	PROB DST. ω_H
NORMALIZATION	$\text{Tr}(\rho) = 1$	$\int \omega_H d\gamma_H = 1$
OBSERVABLE	A... OPERATOR	A(p,q)... PHASE SPACE F.
EXP VALUE/AVERAGE	$\langle A \rangle = \text{Tr}(\rho A)$	$\langle A \rangle = \int A \omega_H d\gamma_H$

b) LIIOVILLE'S EQUATION

$$\frac{\partial \rho}{\partial t} = \{H, \rho\}$$

LIIOVILLE'S EQ.

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$$\frac{\partial \rho}{\partial t} = \{ H, \rho \}$$

LIIOVILLE'S EQ.

$$\frac{d\rho}{dt} = \{ \rho, H \} + \frac{\partial \rho}{\partial t} = 0$$

CONSEQUENCE OF
UNITARITY OF QM.

1 POSSIBILITY:

$$\rho = \text{CONST}$$

MICROCANONICAL ENSEMBLE

POSSIBILITY 2

$$\begin{aligned} \Omega &= \Omega(\text{CONSERVED QUANTITIES}) \\ &= \Omega(E, \underbrace{\vec{p}, \vec{L}}_{\text{CAN BE REMOVED}}) = \Omega(E) \end{aligned}$$

• CONSIDER TWO SYSTEMS

$$\Omega_1 \Omega_2 = \Omega_{\text{TOT}}$$

$$\log \omega_1 + \log \omega_2 = \log \omega_{\text{TOT}}$$

$$\frac{\omega_1}{e^{\beta E_1}} + \frac{\omega_2}{e^{\beta E_2}} = e^{\beta E_{\text{TOT}}} = e^{\beta (E_1 + E_2)}$$

$$\Rightarrow \boxed{\omega = e^{\beta E}}$$

GIBBS DISTRIBUTION FOR
CANONICAL ENSEMBLE

C) GIBBS DISTRIBUTION

DEF: STATISTICAL (VON NEUMANN) ENTROPY

$$S = -k_B \text{Tr}(\rho \log \rho)$$

PRINCIPLE OF MAXIMAL MESS DENSITY MATRIX ρ
REPRESENTING THE EQUILIBRIUM STATE OF A MICROSYSTEM
MAXIMIZES STAT ENTROPY, SUBJECT TO MACROSCOPIC CONSTRAINTS

CONSTRAINTS:

$$a_i = \ln(\eta A_i), \quad \ln \eta = 1$$

$$I = S - \sum_i \lambda_i (\ln(\eta A_i) - a_i) - \lambda_0 (\ln(\eta) - 1)$$

LAGRANGE MULT.

$$0 = \delta I = -\ln(\delta \eta \log \eta + \delta \eta) - \sum_i \lambda_i \ln(A_i \delta \eta) - \lambda_0 \ln(\delta \eta)$$

$$= \ln(B \delta \eta), \quad B = -\log \eta - 1 - \lambda_i A_i - \lambda_0 = 0$$
$$-1 - \lambda_0 - \sum_i \lambda_i A_i$$

$$\boxed{B=0}$$

TRUE

$$\eta = \ell$$

• IMPOSING $T_{\text{eq}} = 1 = \frac{e^{-1-\lambda_0 T_{\text{eq}}}}{\sum_i e^{-\lambda_i A_i}}$

$$S = \frac{-\sum \lambda_i A_i}{Z}, \quad Z = \sum e^{-\lambda_i A_i}$$

↓ ↓

GIBBS DISTRIBUTION PARTITION FUNCTION

3 IMPORTANT PROPS:

$$a_i = - \frac{\partial \log Z}{\partial \lambda_i}$$

$$S = \sum_i \lambda_i a_i + \log Z$$

$$\lambda_i = \frac{\partial S}{\partial a_i}$$

PROOF: $-\frac{\partial \log Z}{\partial \lambda_i} = -\frac{1}{Z} \frac{\partial Z}{\partial \lambda_i} = -\frac{1}{Z}$

PROOF:
$$-\frac{\partial \log Z}{\partial \lambda_i} = -\frac{1}{Z} \frac{\partial Z}{\partial \lambda_i} = -\frac{1}{Z} \text{Tr} \left(\frac{\partial}{\partial \lambda_i} \underbrace{e^{-\lambda_j A_j}}_{-A_i e^{-\lambda_j A_j}} \right)$$

$$= \text{Tr} \left(A_i \frac{e^{-\lambda_j A_j}}{Z} \right) = \text{Tr}(\rho A_i) = \underline{a_i}$$

SPECIAL CASE: CANONICAL ENSEMBLE ($A_i = H$)

$$U = \langle H \rangle = -T \ln(\mathcal{Z})$$

$$\mathcal{Z} = \frac{\sum e^{-\beta H}}{\mathcal{Z}}, \quad \mathcal{Z} = \text{Tr} e^{-\beta H}$$

LAGRANG. MULT.

CONNECTION TO TDS

1ST LAW: $\delta U = \delta Q + \delta W$

↑ ↑ ↑
ENERGY HEAT WORK

ENERGY

HEAT

$\delta U = T \ln(\delta g H) + T \ln(\delta \epsilon H)$

CHANGES PROB,

MOVES ENERGY LEVELS

HEAT

WORK

TD-TDS

$$dU = \delta Q + \delta W$$

↑ HEAT ↑ WORK

$$(\delta gH) + \boxed{T \ln(\delta gH)}$$

MOVES ENERGY LEVELS

WORK

2ND LAW: CLAUSIUS RELATION

$$\boxed{\delta Q = T \delta S}$$

$$S = -T \ln \Omega$$

$$\delta S = -T \ln(\delta \Omega \log \Omega + \delta \Omega) = -T \ln(\delta \Omega (-\beta H - \log Z) + \delta \Omega)$$

$$= \beta T \ln(\delta \Omega \Omega) + T \ln(\Omega \delta \Omega) = \beta \delta Q$$

$$\Omega \ln \delta \Omega$$

↑ NUMBER

$$\Rightarrow \boxed{\beta = \frac{1}{T}}$$

↓ TEMPERATURE

$\delta U = T \ln(\delta q_H) + T \ln(\delta q_C)$

ENERGY ↑ HEAT ↑ WORK ↑

CHANGES PROB. MOVES ENERGY LEVELS

HEAT WORK

δp_{int} δl_{int}

$$\boxed{F = -T \log Z} \quad \text{FREE ENERGY}$$

$$S = \beta U + \log Z$$

$$ST = U - \underbrace{(-T \log Z)}_F$$

$$\boxed{F = U - TS}$$

$$Z) + \log)$$

Q

$$\frac{1}{T}$$

TEMPERATURE