#### ADVANCED STATISTICAL PHYSICS

#### Lecture 1: Fundamental Concepts - Part I

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#### COURSE CONTENT

#### · Part I : Fundamental Concepts - 2Lec, 1Ex-

- 1. Start with what, why and how.
- 2. Quick review on statistical thermodynamics.
- 3. Crash course on statistical mechanics.

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#### • Part II : Phase Transitions and Critical Phenomena. - 3Lec, 1Ex-

- 1. How phase transitions occur in principle ?
- 2. How phase transitions occur in practice ?
- 3. The Ising model.

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#### · Part III : Quantum Phase Transitions. - 3Lec, 1Ex-

- 1. The condensed matter way of handling quantum phase transitions.
- 2. Quantum phase transitions from a quantum information perspective.

· Part I : Fundamental Concepts.



· Part II and III : Classical and Quantum phase transitions





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Online courses on statistical mechanics :

- ICTP Statistical Mechanics A. Schadicchio, M. Masili. Youtube
- Statistical Mechanics Leonard Susskind. Theoretical Minimum

### PART I : FUNDAMENTAL CONCEPTS

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- A hard task because of the many interactions present in these systems. It is impossible to keep track on many-body systems.
- One strategy is to compute the Schrodinger equation for 10<sup>23</sup> particles. A hopeless strategy
- Another useful way is to look at the collective behavior using basic physical laws.

# And that is the approach of statistical physics.

- 1. Start with what, why and how.
- 2. A review on statistical thermodynamics

#### START WITH WHAT, WHY AND HOW.

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- The complexity of many-body systems is a double-edged sword. It provide a way to fight back.
- Ask a gambler or an insurance agent about when probabilities works ?



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"[A law] is more impressive the greater the simplicity of its premises, the more different are the kinds of things it relates, and the more extended its range of applicability. Therefore, the deep impression which classical thermodynamics made on me. It is the only physical theory of universal content, which I am convinced, that within the framework of applicability of its basic concepts will never be overthrown. "Albert Einstein, quoted in M.J. Klein, Thermodynamics in Einstein's Universe, in Science, 157 (1967), p. 509.

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- It uses probabilities over ensembles.
- Introduction of *a priori* postulates.
- Probability calculations.

### Specification of the state of the system

• Micro-state : a particular configuration a system take at some instant.

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- Example : the Hydrogen atom

The energy levels of the hydrogen atom are given by :  $\epsilon_n = -\frac{-13.6}{n^2}$  eV

The **micro-state** is a particular configuration given by the ensemble  $(n, l, m, s, s_z)$ , which describes the system completely at the microscopic level.

#### CLASSICAL DESCRIPTION : THE NOTION OF PHASE SPACE

Sometimes it is okay to look for help in classical mechanics. Indeed, specifying the position x and the momentum p gives a complete description of systems in classical mechanics.



**Figure 1:** Phase space representation of a one dimensional particle. Each couple of (x, p) is associated to a point in the phase space (i.e. the red point). The time evolution of (x, p) is equivalent to the movement of the point through the phase space.

In quantum mechanics, the wave function  $\psi_k(x_1, \ldots, x_f)$  is the key tool to describe the particles, where f is the number of degrees of freedom.

#### EXAMPLE :

The state of a system consisting of a particle having a spin  $s = \frac{1}{2}$ , can be specified by the projection of the spin on the *z*-axis which can take values of  $+\frac{1}{2}$  or  $-\frac{1}{2}$ . In other terms, we say that the particle points either up or down.

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#### Example 1: Flipping coins.



#### EXAMPLE 2: 3 PARTICLES SYSTEM

Consider three fixed particles each having a spin  $s = \frac{1}{2}$  and a magnetic moment along the *z*-axis of  $\mu$  when it points up and  $-\mu$  when it points down. The system interacts with an external magnetic field *H* along the *z*-axis. The energy of a particle is  $-\mu H$  when it points up and  $+\mu H$  when it points down. The state of *i*<sup>th</sup> particle can be specified by the quantum number  $m_i$  (the projection of the spin on the *z*-axis), which can take two values  $m_i = \pm \frac{1}{2}$ . The state of the whole system can be determined by knowing the values of  $m_1, m_2$  and  $m_3$ .

#### EXAMPLE 2: 3 PARTICLES SYSTEM

State index	Ouantum numbers	Total magnetic	Total
r	$m_1, m_2, m_3$	moment	energy
1	+ + +	$3\mu$	$-3\mu H$
2	+ + -	$\mu$	$-\mu H$
3	+ - +	$\mu$	$-\mu H$
4	- + +	$\mu$	$-\mu H$
5	+	$-\mu$	+ $\mu H$
6	- + -	$-\mu$	+ $\mu H$
7	+	$-\mu$	+ $\mu H$
8		$-3\mu$	+3µH

**BASIC POSTULATES** 

## "For an isolated system in equilibrium, all accessible states are equally likely."

## "The mean over time of any parameter is equal to the average of this parameter taken over an ensemble of systems."

#### **PROBABILITY CALCULATIONS**

- Consider an isolated system at equilibrium. Its energy lies between *E* and  $E + \delta E$ .
- Let  $\Omega(E)$  be the total number of state in this range.
- Suppose that among these states there is a certain number  $\Omega(E, y_k)$  of states for which some parameter y (i.e. magnetic field, pressure ) takes the value  $y_k$ .

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Using the equiprobability postulate, we can say the probability  $P(y_k)$  that the parameter y takes the value  $y_k$  is :

$$P(y_k) = \frac{\Omega(E, y_k)}{\Omega(E)}$$

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We can also calculate the mean of this parameter by taking the average over the system in the ensemble :

$$\langle y \rangle = \sum_{k} P(y_k) y_k$$

### A REVIEW ON STATISTICAL THERMODYNAM-ICS

"The history of thermodynamics is a story of people and concepts. The cast of characters is large. At least ten scientists played major roles in creating thermodynamics, and their work spanned more than a century. The list of concepts, on the other hand, is surprisingly small; there are just three leading concepts in thermodynamics: energy, entropy, and absolute temperature." William H. Cropper

#### Zeroth Law :

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If two systems A and B are in thermal equilibrium with a third system C, then A and B are in thermal equilibrium with each other. FIRST LAW :

An isolated system at equilibrium is characterized by a macro-state which has a constant internal energy  $\overline{E}$  =constant. If the system is allowed to change macrostates (not isolated), the change in the internal energy is given by :

$$\Delta \bar{E} = -W + Q,$$

where -W is the work done by the system and +Q is the heat absorbed by the system.

#### SECOND LAW :

In any thermodynamic process, the total entropy "S" either increases or remains constant, but never decreases.

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#### THIRD LAW :

The entropy "S" has a limiting property that : as  $T \rightarrow 0_+$ ,  $S \rightarrow S_0$ . Where  $S_0$  is a constant independent of all the parameters of the system. Consider a closed system composed of two parts A and B, the thermodynamical variables of the whole system (E, V, N), obeys the following :  $V = V_1 + V_2$ ,  $E = E_1 + E_2$  and  $N = N_1 + N_2$ .

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at constant N and E: 
$$\left(\frac{\partial S_1}{\partial V_1}\right) = \left(\frac{\partial S_2}{\partial V_2}\right) = \frac{P}{T}$$
,  
at constant V and N:  $\left(\frac{\partial S_1}{\partial E_1}\right) = \left(\frac{\partial S_2}{\partial E_2}\right) = \frac{1}{T}$ ,  
at constant E and V:  $\left(\frac{\partial S_1}{\partial N_1}\right) = \left(\frac{\partial S_2}{\partial N_2}\right) = -\frac{\mu}{T}$ .

heat capacity at constant volume : 
$$C_V = T \left( \frac{\partial S}{\partial T} \right)_V$$
,

heat capacity at constant volume : 
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heat capacity at constant pressure : 
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heat capacity at constant pressure :  $C_P = T \left(\frac{\partial S}{\partial T}\right)_P$ .

The internal energy is :  $dE = TdS - PdV = \delta Q + \delta W$ ,

The concept of *"the enthalpy"* and *"the free energy"* (which will be central to the analysis of phase transitions later on), can be defined :

$$H = E + PV = TS + \sum_{j=1}^{r} \mu_j N_j$$
$$dH = TdS + VdP + \sum_{j=1}^{r} \mu_j N_j$$

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$$dH = TdS + VdP + \sum_{j=1}^{r} \mu_j N_j$$

$$F = E - TS = -PV + \sum_{j=1}^{r} \mu_j N_j,$$
$$dF = -SdT - PdV + \sum_{j=1}^{r} \mu_j N_j$$

## THERMODYNAMICS FROM STATISTICAL RE-

Our starting point is the entropy, a concept that precedes the temperature and even the energy. Consider a closed system of N particles at equilibrium; if  $\Omega(N, E, V)$  is the total number of configurations, then the equiprobability postulate states that the probability of finding the system in any of its accessible states is :

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Then :

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and :

$$\beta = \frac{1}{k_b T} = \frac{\partial \ln \Omega(N, E, V)}{\partial E}$$

#### THERMODYNAMICS FROM STATISTICAL RELATIONS

EXAMPLE : IDEAL GAS

$$\Omega^{\text{Ideal gas}}(N, E, V) \propto V^N f(E),$$

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 $\ln \Omega = N \ln V + \ln f(E) + \text{constant},$ 

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Thus, it follows that, for an ideal gas  $\beta = \beta(\overline{E})$  or  $\overline{E} = \overline{E}(T)$ . The mean energy of an ideal gas depends solely on the temperature.

# Thank you for your attendance and attention.