

Lecture 1

First day information

- 1) syllabus
- 2) website/D2L → lecture notes
- 3) course structure - HW  
- Exam days
- 4) Assignments - HW typically due Tues and Friday. → late policy.  
- exam dates in syllabus
- 5) Key access
- 6) Search candidates
- 7) SPS?

Assignments HW 1 by Friday 5pm

Thurs : read 2.4, 2.5

2.22 (first part)

Introduction to Statistical and Thermal Physics

Thermal and statistical physics considers physical systems which contain a large number of identical or similar individual constituents. Rather than describe the behavior of individual constituents we aim to describe the entire system in bulk.

Consider two examples:

- 1) gas consisting of molecules
- 2) collection of nuclear spins.

## Example: Gas consisting of molecules

### Demo: PhET Gas Properties

- \* insert 100 heavy/one light
- \* try to track light particle.
- \* observe well define bulk variables:  $P, V, T$

We could aim to track each individual particle using classical physics. This would require tracking the position and momentum of each particle as time passes. However this would not necessarily yield any insight about the system's state or behavior. Nor would it necessarily be amenable to experimental verification.

However, we can track the overall behavior of the system using bulk variables such as pressure, volume and temperature. We would like to, amongst others, describe as precisely as possible how these are related.

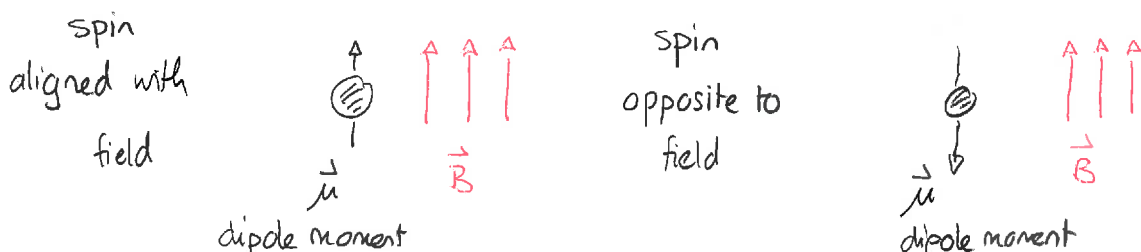
We can also track the statistical behavior of quantities such as molecular speeds or energies. - Demo PhET Gas Properties Energy Tab.  
How are these aspects of the system's behavior related?

## Example: Nuclear Spin Ensemble

### Demo: PhET Simplified MRI

- \* Simplified NMR tab
- \* Power at 75%
- \* Keep frequency fixed - adjust main field to achieve resonance.

A nuclear spin is a type of magnetic dipole (atomic scale compass) that is inherent to certain nuclei. Such spins can interact with external magnetic fields. Quantum physics then describes two preferential (energy) states:



The state of any individual spin can be described by stating whether it is aligned or opposite to the external field. The animation suggests that for a large collection of such spins that are not interacting, some will be in the up state and others in the down state. Again we do not aim to describe this. Rather we aim to describe the bulk magnetization:

$$\vec{M} = \sum \text{individual dipole moments } \vec{\mu}$$

and how this depends on the external magnetic field, the temperature of the surrounding environment and so on.

A quantity of this type can routinely be measured in NMR or MRI experiments. We can also ask about the fraction of nuclei in one state or equivalently the probability with which any nuclei is in either state.

How are such statistical properties related to bulk magnetic properties?

These two examples illustrate some basic ideas from thermodynamics and statistical physics. Thermodynamics aims to describe bulk properties of systems and give a scheme for relating this, particularly during processes where the system state changes.

Statistical physics considers possible microscopic states of such systems and addresses the issue of how likely they are. Ultimately it provides a scheme for extracting relationships between bulk properties.

### Thermodynamics: A general framework

The two examples illustrate very different types of system. Thermodynamics will provide a unifying description for all such systems. There will be two common mathematical quantities for all thermodynamic systems:

- 1) system energy:  $E$
- 2) system entropy:  $S$

These will be constructed in different ways for various systems but the same basic rules will apply. For example, the temperature of any system can always be found using:

$$\frac{1}{T} = \frac{\partial S}{\partial E}$$

We aim to develop such rules and apply the resulting science to a wide range of physical systems. Examples include:

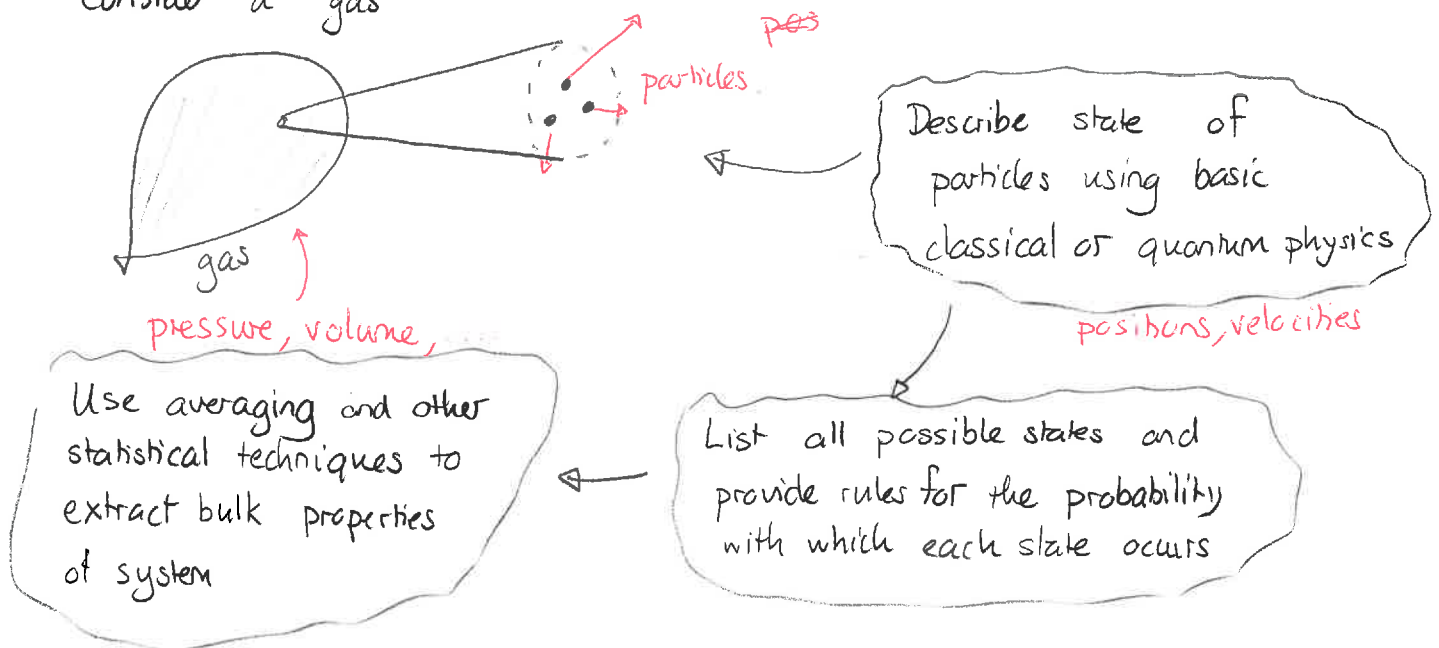
- condensed matter / solid state physics
- chemistry
- astrophysics
- nuclear physics

list on pages 1,2

### Statistical Physics: A general framework.

Thermodynamics gives relationships between bulk quantities such as, for an ideal gas,  $PV = NkT$ . We can ask how these emerge from the physical properties of the system constituents. Statistical mechanics addresses this.

Consider a gas



Texts: Website lists various texts. There are many approaches.

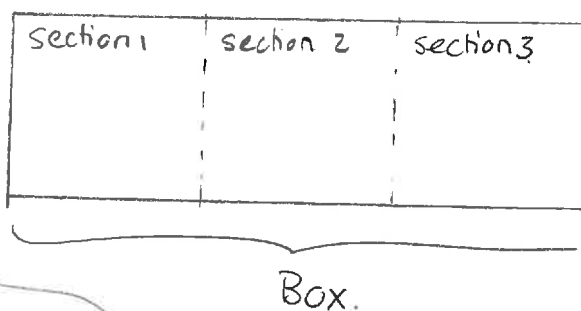
## Statistical physics: toy models

The key ideas in statistical physics can be illustrated via extremely simplified "toy" models. These include:

- 1) coin toss
- 2) particle in subdivided boxes

Consider particles that can inhabit a box. Suppose that the box has three sections. We place  $N$  particles into the box and shake them. We can ask how

they will be distributed subsequently. To do this we can represent the state of the system by:



$N$  = total number of particles

$n_j$  = number of particles in section  $j$

Specifying values for  $N, n_1, n_2, n_3$  then specifies the state of the system. Note that there is a constraint:

$$n_1 + n_2 + n_3 = N.$$

We can now address questions such as:

- 1) after many interactions between particles does  $n_1$  approach a fixed value? If so, what? What about  $n_2$ ?
- 2) can we describe and predict an "equilibrium state" for this system?

We can illustrate this with an animation.

Some homework problems and class exercises will use simulations developed by the text authors. These can all be run from a java “launcher.” You should first install the launcher on the computer that you are using. To do this:

1. Go to the following webpage: <http://www.compadre.org/STP/items/detail.cfm?ID=7308>.
2. Download the file called “download 3239kb.jar.” You may have to save it and then run it.

Running the file produces a “launcher” window (with the tab title Open Source Physics: osp\_stp.xset) which lists a long collection of simulations for statistical and thermal physics these are sorted into folders in the directory on the left. Double click on any entry to run the relevant simulation.

General tips about running the simulations:

1. Clicking on a simulation in the “launcher” will produce documentation for the simulation in the launcher window.
2. The “launcher” usually opens a controller window but not necessarily the other windows associated with the simulation. The controller window lets you set parameters. Once you have done this clicking Initialize will open the simulation usually with some other graphical windows. Clicking Start will actually run the simulation.
3. Graphs and images can be save by following Tools → Snapshot ...
4. The data that is generated by the simulation can be accessed in tabular form by following Tools → Data Tool, selecting one of the starred objects and clicking OK. This contains a Statistics button that will computer averages and deviations. Data that goes into such a calculation can be selected by highlighting the relevant entries in the columns.

## 1 Approaching equilibrium

Launch “Approach to equilibrium → Three partitions.” The LJgasApp controller appears. Set the number of particles to 270 and click “Initialize.” This will produce a box with three subdivisions and all particles initially in the middle subdivision. The particles can collide and move across the subdivisions.

- a) If the boundaries for the middle subdivision are removed, how many particles do you expect will eventually be in each subdivision? Do you expect this number to be exact?
- b) Run the simulation for 60s and observe the graph of the number of particles in each cell. Do these appear to approach fixed values? Do these agree with your previous answer?
- c) To determine the exact numbers in the graph follow, Tools → Data Tool → DataSet 1, 2, 3 and click OK. Determine the number of particles in each cell at  $t = 2$ ,  $t = 10$  and  $t = 20$ . Determine the average from  $t = 20$  to  $t = 40$ ; this requires highlighting and using the Analyze tab. Repeat this for  $t = 40$  to  $t = 60$ .
- d) Is the system initially in an equilibrium state? Does it approach an equilibrium state? Which of the data that you extracted can you use to describe equilibrium?
- e) Are there fluctuations in the variables used to describe the state of the system? Do you expect that these will be more or less pronounced as the number of particle increases?

Exercise

Class discussion

Answer:

- a) One might expect  $\frac{1}{3}$  in each section  
 $\Rightarrow$  90 per section

These will probably fluctuate

- b) They all appear to reach somewhere around 90. There are fluctuations.

c)

t	$n_1$	$n_2$	$n_3$
2	57	155	58
10	88	105	77
20	93	94	83

averages

t range	$\bar{n}_1$	$\bar{n}_2$	$\bar{n}_3$
20-40	89.11	91.61	89.28
40-60	91.03	90.78	88.19

$\updownarrow$  similar

- d) No - the values of  $n_1, n_2, n_3$  never approach this

Yes - it approaches about 90 per section on average.

The mean number in each section describes equilibrium

- e) Yes the data shows this.

Probably less pronounced as number increases.

Demo: Try with 2700

The model is primitive but illustrates some features of statistical systems.

These include:

- 1) the average statistical behavior of such systems can be described
- 2) one can use statistical behavior to describe equilibrium
- 3) as the size of the system grows statistical fluctuations become less important.

We will eventually convert this into a mathematical model with predictive possibilities



# Thermodynamics: Overview

Thermodynamics gives a method and language for describing the bulk properties of any system with multiple constituents. We will typically illustrate this using gases but the basic concepts apply to many other systems such as spin-1/2 particles, oscillating nuclei in a solid, ...

Consider a gas:

1.

Describe the system and its possible states by listing bulk variables

system



- type of gas  
(e.g. ideal)

- variables

$P, V, N, T, E, \dots$

2.

Relate the variables that describe the system. This gives equations of state

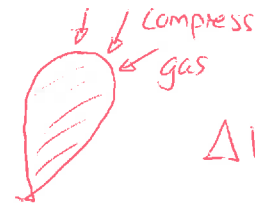
e.g. ideal gas

$$PV = NkT$$

$$E = \frac{3}{2}PV$$

3.

Consider processes where the state of the system changes. Describe these using energy



$$\Delta E = W + Q$$

First law

4.

Describe processes that are possible for interacting systems

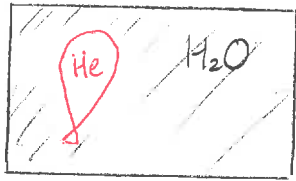


$$\Delta S \geq 0$$

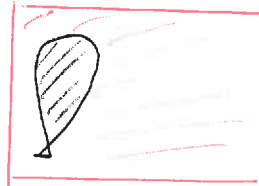
Second Law

## Systems and states

There will usually be many possible candidates for "the system" in a thermodynamic situation. Consider a balloon filled with Helium that is immersed in water. There are at least three possibilities:



system = Helium gas  
environment = water



system = water  
environment = Helium gas



system = Helium gas  
AND water

We always need to specify the system clearly. In some situations we delineate system and environment apply laws of thermodynamics to both and deduce special rules for the system alone.

We next need to describe states of the system. There are two steps

List bulk variables  
that can describe  
any state

Specify particular values  
for each variable in order  
to specify a particular  
state for the system

## Thermodynamic states for a gas

We illustrate the process for a gas. Possible relevant bulk variables are:

$N$  = Number of molecules → count molecules

$V$  = Volume of gas → measure dimensions / calculate

$P$  = Pressure of gas → same everywhere  
→ force/area on sides

$T$  = Temperature of gas → Thermometer?  
Precise definition?

Additional possibilities are:

- molecular mass
- molecular dipole moment, ...

### Demo: PhET Gas Prep

- \* Inject molecules
- \* list states

	N	V	P	T
state 1	100	original	11.6atm	300K
state 2	100	half orig	23.5atm	300K
state 3	200	original	23.5atm	300K

same T but  
different P  $\equiv$  NOT  
equiv.

We note:

- 1) equivalent states - two states are equivalent if the value for each variable is the same between the states.
- 2) equilibrium states - require one value of P throughout gas,  
one value of T " "  
- cannot describe sudden changes since variables are clearly not the same at different locations in system. DEMO - compress old PhET
- 3) fluctuations. - there will be fluctuations in some variables  
- with large enough numbers of constituents, these fluctuations are negligible.