Welcome

* syllabus
* Website / Lecture Notes
* D2L page info
* Course structure / deliverables – HW twice per week
  – Exam dates

Other

* Key access

This Week HW 1 by Friday 5pm

Thurs: Read 2.4, 2.5

Introduction

Statistical and thermal physics considers physical systems that contain a very large number of identical or similar constituents. Rather than describe the behavior of individual constituents we aim to aggregate their individual properties into bulk quantities that describe the entire system.

We illustrate this for two very different types of system:

1) a gas consisting of molecules
2) a collection of spin-½ particles.

Example Gas

DEMO: PhET Gas Properties → Ideal

* Insert 200 heavy, 1 light
* Can we track light particle?
* Are there variables to describe the gas that stay roughly constant?

Classical physics promises that we could track the trajectory of each individual particle, such as the lighter particle. This would require the position and momentum of each molecule as a function of time. However, even with precise data for all molecules it is not necessarily clear that it gives any insight into the overall behavior of the gas. Nor could we check the predictions easily experimentally.

But we can see that it is possible to track the overall behavior of the gas in terms of bulk variables: volume, pressure, temperature, ...

We would like to use these to describe the gas and relate them to each other.

DEMO: PhET Gas Properties – Energy

* Insert 200 molecules
* Observe distribution of
  - speeds
  - kinetic energies

We could also hope to describe statistical properties of the gas molecules:

* how are speeds or energies distributed?

Eventually we aim to relate

Statistical properties of molecules ⟷ Bulk gas variables

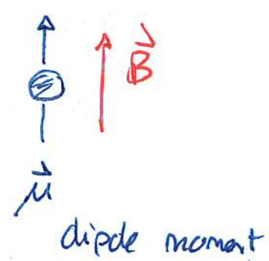
Example Nuclear Spins

DEMO: PhET Simplified MRI

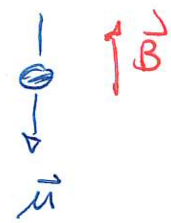
* Simplified NMR Tab
* Power at 75%
* Fix frequency
* Adjust main field $\rightsquigarrow$ resonance

A nuclear spin is a type of magnetic dipole (atomic scale compass) inherent to certain atomic nuclei. These spins can interact with external magnetic fields. These interactions are described using quantum theory. There are two preferential states of energy

spin aligned with field



spin opposite to field.



When the spins are not interacting, we see that some are aligned and others are opposite. We can ask:

* what fraction are aligned?
* what bulk quantity can we measure to describe the bulk state of the collection of spins
* how are these related to temperature?
* how do these change if energy is added?

These are routine considerations in NMR and MRI. Thermal and statistical physics provides methods for assessing such collections of nuclear spins.

Thermodynamics: a general framework

The two examples are very different types of systems and at the microscopic level the basic physics is very different.

However, thermodynamics will provide one framework that can describe both of these and other bulk systems. There will be two common mathematical quantities:

1) total system energy: E
2) total system entropy: S

Their construction will depend on the system. However, they will yield some very general rules. For example the temperature can always be determined by

$$T = 1 \Big/ \left(\frac{\partial S}{\partial E}\right)$$

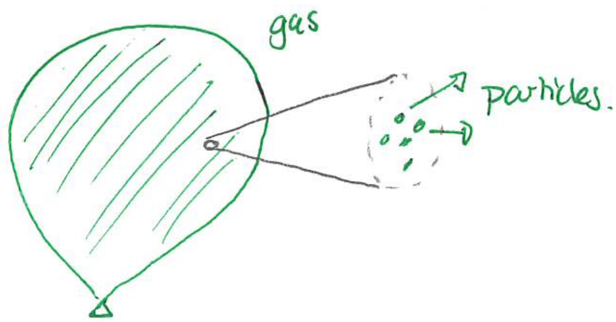
We will provide the basic framework of thermodynamics. It can be applied to a wide range of sciences:

- condensed matter / solid state physics
- chemistry
- astrophysics

see pages 1→2

Statistical physics: a general framework

Statistical physics provides a method for connecting microscopic descriptions of systems to bulk thermodynamic quantities.



Describe states of individual constituents. Use classical or quantum theory

e.g. position, momentum of each particle

List all <u>possible</u> states of individual constituents. Provide rules for the probability with which each state occurs

Use averaging and other statistical techniques to extract bulk variables for system

e.g. Pressure, volume, temperature

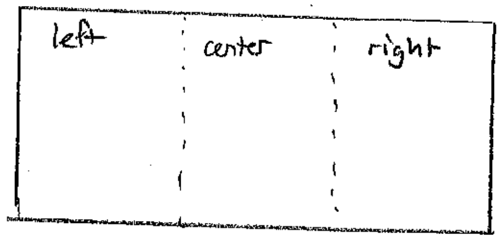
Toy models

We can illustrate the basic ideas of statistical physics via very simplified "toy" models. Examples include:

1) coin toss
2) particles in subdivide boxes.

Consider particles that can inhabit a box which is subdivided into three sections. Let

N = total number of particles in box



We can allow the particles to move (or shake them) and then ask how many there will be in each section. Let

n_{right} = number in right
n_{center} = " " center, ...

- We ignore the identities of the individual particles - we cannot see these. Then the state of the system is described by specifying values for: N, n_r, n_c, n_ℓ

We note a constraint:

$$n_\ell + n_c + n_r = N.$$

We can ask

1) after many interactions does n_ℓ approach a fixed value? If so, what? What about n_c?
2) can we describe and predict an "equilibrium state" for this system?

Some homework problems and class exercises will use simulations developed by the text authors. These can be found at the website Statistical and Thermal Physics Programs. The simulations are run from a web browser.

Clicking on a particular program provides a "controller" window which allows you to control the program. The output will appear in a separate window inside the browser.

General tips about running the simulations:

1. The controller window lets you set parameters. Clicking Initialize will open the simulation usually with some other graphical windows. Clicking Start will actually run the simulation.

2. The data that is generated by the simulation can be accessed in tabular form by following Tools → Data Tool, selecting one or more of the starred objects and clicking OK. This contains an Analyze option that allows access to the statistics 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

From the program website, follow STP Programs → Thermal Physics → Three Parts MD. 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 60 s 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 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 option. 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?

Answer:

a) About one third in each. So about 90 per section

b) The appear to fluctuate around 90.

c)

t	n left	n center	n right
2	65	147	58
16	89	97	84
20	93	88	89.

averages

t range	left	center	right
$20 \to 40$	93 ± 3	90 ± 3	87 ± 4
$40 \to 60$	92 ± 4	92 ± 5	85 ± 6

d) No, the values for n left, n center and n right never approach close to the initial state.

It looks like it approaches an equilibrium state of ~90 per section.

The mean number describes equilibrium.

e) Yes (the standard deviations). Probably less pronounced

DEMO: Show this with about $N = 900$

This is a simplistic model but it can illustrate some features of statistical systems.
For example:

1) one can describe the average behavior of such systems accurately
2) one can describe equilibrium circumstances statistically
3) as the system size increases fluctuations become less important.

We will develop a mathematical model with these features that can describe physical systems.

Thermodynamics Outline

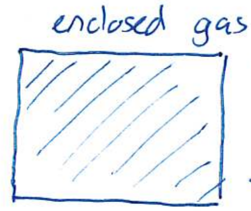
Thermodynamics provides a coherent robust framework for describing bulk systems. We will illustrate it's features using gases. However, be aware that the concepts apply far more generally than gases and eventually encompass:

1) systems of spin-½ particles
2) oscillating nuclei in solids
3) collections of photons ...

Considering a gas, the framework is:

1. Describe the type of system and its possible states by listing bulk variables.

e.g.



— what type of gas: e.g. ideal monoatomic

— variables $P, V, T, N, E, \ldots$

2. Relate the variables that describe the system. This gives <u>equations of state</u>

e.g. for an ideal monoatomic gas

$$PV = NkT$$

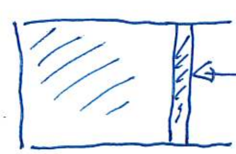
$$E = \frac{3}{2}NkT$$

3. Describe ways in which the variables can be measured and how these determine equations of state

e.g. thermal expansion coefficient $\frac{\partial V}{\partial T}$

e.g. heat capacity $C = \frac{\partial E}{\partial T}$

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



e.g. compress gas.

$\Delta E = Q + W$ First Law

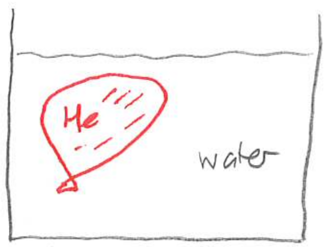
5. Describe processes that are possible for interacting systems

Second Law

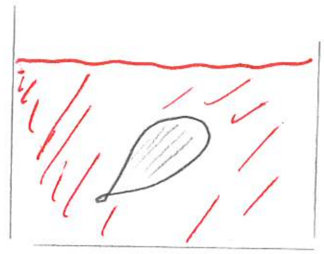
$$\Delta S \geq 0$$

Systems and states

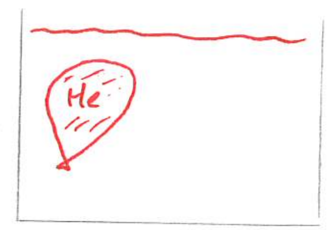
We need to specify the system that we consider. Although there are many valid choices, we must specify what we mean by "the system." Consider a balloon filled with Helium that is immersed in water. Possibilities for the system are:



system = He gas
environment = water



system = water
environment = He gas



system = helium gas AND water.

Sometimes we apply the laws of thermodynamics to the system and environment and then use these to deduce special rules for the system alone.

The next step is to describe the state of the system. This is done in terms of quantities or variables. The process is:

List bulk <u>variables</u> that can describe system $\longrightarrow$ Specify particular values for each variable. A list of such values specifies <u>one state</u> of the system

Thermodynamic states for a gas

The description of states can be illustrated by a gas. The relevant possible bulk variables are:

N = number of molecules $\longrightarrow$ count molecules

V = volume of gas $\longrightarrow$ measure dimensions and use geometry to calculate volume

P = pressure of gas $\longrightarrow$ same <u>everywhere</u> $\equiv$ force / unit area

T = temperature of gas $\longrightarrow$ measure with a thermometer? better definition?

We could entertain additional possible variables: e.g.

- molecular mass
- molecular electric dipole moment
- nuclear spin state..

DEMO: PhET Gas Properties

* inject molecules
* list states

	N	V	P	T
state A	100	original	11.5 atm	300K
state B	100	half original	23 atm	300K
state C	200	original.	23 atm.	300K

Same T, different P
DIFFERENT states

Then:

1) equivalent states - two states are equivalent $\Leftrightarrow$ the value for each variable is the same between the states

2) equilibrium states - each variable has one value for the entire system

e.g. one value of P, one value of T throughout

- we cannot describe sudden changes since the variables will differ at various locations at the same time.

$\hookrightarrow$ DEMO rapid expansion

3) fluctuations

- some variables will fluctuate
- with a large number of constituents, these are negligible.