October 22, 2023.
JGU Mainz
Course 08.128.140., WiSe 2023/24.
Theoretische Physik 4. Statistische Physik.

Dr. Felix Yu (fyu001@uni-mainz.de)

Lecture 1.

Course administration.

The course assistants for this term are
Lucas Heger, Riccardo J. Valencia Tortora,
+ Emanuele Zippo.

Lecture notes, homework sheets, homework solutions,
+ other course materials will be
posted online on Moodle.

Discussion sessions will start the second week
of the semester.

Tues. 2-4pm (c.t.) – Seminar room F, Lucas (Deutsch)
Wed. 10-12pm (c.t.) – Seminar room A,
Wed. 2-4pm (c.t.) – Seminar room A,

Homework is due each week on Monday in class.
Exam eligibility: 50% of total HW credits.
Exam 1: March 1, 2023, 9-12pm (s.t.)
Exam 2: March 27, 2023 9-12pm (s.t.)

Main textbooks: Kardar ; Blundell + Blundell.
Both available as e-books on university network.
Office hours: by email appointment.

Course outline: 4 units.

Thermodynamics
Probability & statistics
Classical statistical mechanics
Quantum statistical mechanics.

We begin with an introduction & motivation to the course.

There are several avenues and trains of thought that motivate or lead to the development of statistical methods as applied to physics problems. We will illustrate several examples in turn.

① Consider $\vec{F} = m\vec{a}$. From this equation, we can apply a force $\vec{F}$ on some object and observe a corresponding acceleration $\vec{a}$; given the force and acceleration are always aligned in the same direction, we can ascribe the proportionality constant between $\vec{F}$ and its resulting $\vec{a}$ as a scalar (pure number) quantity which we ~~[illegible]~~ call an object's mass m.

Taking this equation at face value, we can consider many individual ~~[illegible]~~ force instead of a collective single ~~[illegible]~~ force. For example, rain falling on a roof exerts collective force at any given instant in time, but the individual / granular information about how many raindrops are falling at any given instant is not necessary to understand the collective / aggregate force. Moreover, the aggregate force on the roof grows with the area of the roof, and so it is natural to divide out the area and ~~express~~ discuss the pressure exerted by the collective (and stochastic) behavior of the raindrops, $\vec{p} = \frac{\vec{F}}{A}$. Note that implicitly we are all also doing an average in the time domain as well an average in the roof surface to ~~meaningf~~ meaningfully define pressure $\vec{p}$: from one instant to the next, the distribution of ~~s~~ the number of raindrops in time is varying in a (more or less) random fashion ~~but~~ and the distribution of raindrops across the surface of roof (vs. just missing the roof) is also varying randomly. Nevertheless, for some suitably defined averaging procedure constructed on the granular & microscopic action of the raindrops, the mean = average behavior of the rain as a pressure force is suitable for describing the system.

From ~~s~~ here, we can note a few facts about the central concepts ~~s~~ ~~the~~ underlying the opposite approaches between thermodynamics and statistical mechanics.

Thermodynamics starts with aggregate quantities to describe the behavior of a system from a phenomenological approach.

Statistical mechanics, on the other hand, builds a (terrifyingly & inordinately unwieldy) microscopic enumeration of the possible states of a system and then uses statistical (i.e. averaging) methods to derive the macroscopic behavior of the system.

Why is the microscopic enumeration so inordinately unwieldy?

(2) Consider a gas of non-interacting atoms in a box. A typical number of atoms in every day experience is Avogadro's number, $A = 6.022 \cdot 10^{23}$, since a 12 g sample of Carbon 12 has A number of carbon atoms. If each atom is labeled by its (x, y, z) position in the box and also by its velocity (v_x, v_y, v_z), then we have $6A$ data points to keep track of at any given time. Finding a suitable reduction in complexity of the microscopic degrees of freedom necessarily coincides with defining a microscopic origin of the thermodynamic variables mentioned earlier. This again leads to a statistical approach where the properties of the system are derived from an appriate average of the microscopic degrees of freedom.

(3) Another conceptual approach that leads naturally to statistical mechanics is the concept of statics vs. dynamics in physics. In particular, a dynamical change to a system, like a force of a piston in a car engine,

can always be modeled as the change in some total quantity weighted by corresponding conjugate variable: in other words, a differential relationship. If there are multiple variables (microscopic quantities) that feed into the total quantity, then even an overall dynamical change in the system has <u>degeneracies</u> in how it is expressed in terms of microscopic degrees of freedom. As an example, the total kinetic energy of N gas particles (non-relativistic) is $E_{tot} = \sum_{i=1}^{N} \frac{1}{2} m_i |\vec{v}_i|^2$

where $|\vec{v}_i|$ is the magnitude of the 3-velocity. For a given particle, swapping $v_{ix} \leftrightarrow v_{iy} \leftrightarrow v_{iz}$ will keep its kinetic energy unchanged, and so there are many different configurations of velocities of the N particles that would share the same total kinetic energy.

If the system is isolated, i.e. no new energy is added or subtracted, then elastic interactions among the particles can change individual $\vec{v}_i$ but will keep E_{tot} unchanged. (We will see that this results in a Maxwell-Boltzmann distribution of velocities.). How does the system equilibrate? We can use intuition that if some (macroscopic or microscopic) part of the system has an <u>average</u> kinetic energy that is higher than the ensemble average, then probability (via the elastic collisions among the gas particles) will require this collection to swing to an "opposite" lower average kinetic energy at some later time. The fact that this happens across multiple spatial + time domains, according to laws of probability, is the essence of a system in equilibrium. It is important to note that a microscopic overfluctuation or underfluctuation is both allowed + expected.

If the system is coupled to an external reservoir (where some macroscopic variable such as temperature, pressure, etc.) is different, then the system as a whole behaves as a probabilistic ensemble but with a bias. The timescale of changes to the macroscopic quantities will then possibly compete with the intrinsic timescales of changes in the microscopic quantities.

We remark that a central feature of statistical methods applied to large numbers is the fact that single outliers make essentially no impact on aggregate or average quantities.

Another remark: We should also discuss what is meant by "thermodynamics is a phenomenological model." In the 1800s, the development of thermodynamics was driven by the need to understand engines, heat, gases, work, etc. You can imagine that for studying and developing engines, the scientists would test all sorts of observable properties ~~vary~~ & variations of inputs & measure the outputs with mathematical modeling of the relationship. This is the essence of a phenomenological model → take data & fit the data to an underlying mathematical description.

Two points: ① the underlying mathematical description works by design but is not motivated from first principles. The fact that thermodynamics laws, its postulates & observations arise from stat. mech is a reason to regard stat. mech. as more fundamental.

② Phenomenological models will generally always have a limited regime of validity, since the data gathered will only be informed by inputs varied in a finite range. Thus, the idealization afforded by phenomenological models generally emerge as limiting behavior of fundamental descriptions. When outputs are no longer expressable (think phase changes from gas to solid via changes in pressure) in the same language, a classification by equivalence classes becomes motivated to relate similar regimes.

Next time:

More on equilibrium as a concept.

- time (in)dependence
- adiabaticity

State functions

Extensive & intensive variables.