Lecture 5 - Fundamental postulate

What's Important:
- description of a state
- probability
- density of states

Text: Reif

Secs. 2.1 to 2.5 should be read independently

Description of a state

In *classical mechanics*, a 3D system of N particles without spin or any internal structure can be described by 6N variables.

positions: $\mathbf{q}_1 \ldots \mathbf{q}_N$ (coordinates are the degrees of freedom)
momenta: $\mathbf{p}_1 \ldots \mathbf{p}_N$

Knowing these quantities at a particular time, one can use Hamilton's or Newton's equations to predict their values at all later times. The coordinate variables $\mathbf{q}$ are called the degrees of freedom f of the system. Here, there are 3N coordinates so f = 3N. The positions and momenta of the particles form the *phase space* of the system.

In *spin systems* on a fixed lattice, the degrees of freedom are the spin orientations:

↑↓↓↑↑↑↓↓↓↑↑↓↑↓↑↑ f degrees of freedom

In quantum mechanics, the number of degrees of freedom is the number of quantum numbers required to specify the state. For example:

1 harmonic oscillator	$E = (n + 1/2)\, \omega h / 2\pi$	$f = 1$
N weakly coupled oscillators	$E = (n_1 + n_2 \ldots + N/2)\, \omega h / 2\pi$	$f = N$

Summary A microscopic state or *microstate* of the system is a specified state of
- phase space coordinates
- spin orientations
- quantum numbers.

More than one microstate may have a specified energy (degeneracy).

Accessible states

Out of this potentially large set of states, there exist a set of *accessible states* of the system, specified by a global system characteristic such as the energy. For example, three spin - 1/2 objects in a magnetic field:

congurations			# of accessible states in energy range
	↑↑↑		1
↑↑↓	↑↓↑	↓↑↑	3
↓↓↑	↓↑↓	↑↓↓	3
	↓↓↓		1

A system has a set of accessible states in which it can be found. The fundamental postulate of statistical mechanics is:

An isolated system in equilibrium is equally likely to occupy any of its accessible states.

Notes:
1. *Isolated* means that there is no exchange of energy or particles with other systems.
2. *Equilibrium*: if it's not in equilibrium, some states are more preferred than others and the system will evolve in time.

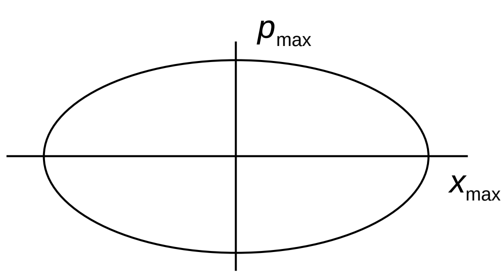
Example:
Consider a classical harmonic oscillator in one dimension. Does the fundamental postulate mean that the oscillator (or an ensemble of isolated oscillators, each with their own phase space) have equal likelihood of having any spatial position x allowed by conservation of energy? **NO**. Why?

The phase space of the oscillator is elliptical, owing to conservation of energy:

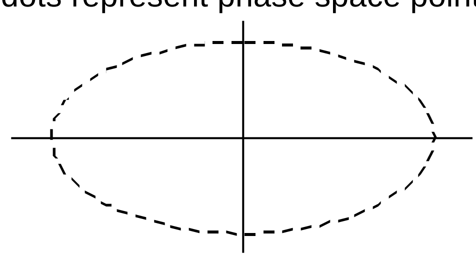
$$E = \frac{p^2}{2m} + \frac{kx^2}{2}$$

or

$$1 = \frac{p^2}{2mE} + \frac{kx^2}{2E} = \left(\frac{p}{p_{max}}\right)^2 + \left(\frac{x}{x_{max}}\right)^2$$



The oscillator is equally likely to be found at any *phase space* point on the trajectory. For example, let the dots represent phase space points



The oscillator has more "dots" at large x (around the classical turning points) than it does near $x = 0$, where it has its greatest speed. Thus, the oscillator is more likely to be found at large x than at $x = 0$.

Probability

Suppose that we have an energy range E to $E + \delta E$, which specifies the accessible states of the system:

¾
¾
¾ $E + \delta E$
¾ define Ω to be the number of states in this region
¾ E
¾
¾
¾

Let's measure the value of an observable y, which we say has discrete values

$y_1\ y_2\ ...\ y_k\ ...$

The number of accessible states with observable y having the value y_k we denote by

$\Omega(E; y_k)$.

By the fundamental postulate, the probability of observing the system with observable y_k is then

[*Prob. of* y_k] = [# *of accessible states with* y_k] / [# *accessible states in total*]

or

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

where

$$\Omega(E) = \sum_k \Omega(E;y_k).$$

To find the mean value of y, we just proceed as usual for all y_k

$$\bar{y} = \sum_k y_k P(y_k) = \frac{\sum_k y_k \Omega(E;y_k)}{\Omega(E)}.$$

Density of states

The discussion above is based upon a discrete counting of states. A continuum description requires a *density of states*, just as a probability density is needed for continuous probabilities:

$\Omega(E) = \omega(E)\,\delta E$ δE = energy range $\omega(E)$ = density of states.

The density of states may be large, and increases rapidly with the number of particles.