Physics 114 **Statistical Mechanics** **Spring 2021**

Week 4 Conceptual Overview

Concept checklist from Readings:

- Prof. David Park of Williams College always told us "*Probabilty* doesn't tell you whether you will win, but it tells you how to play the game." It also tells us how gas molecules, electrons, photons, ... play their games.

- We imagine a space of *exclusive outcomes* of experiments $\{x_i\}$, called the *sample space*. The function $P(x_i)$ represents the likelihood of seeing result x_i upon *one trial* of the experiment. If we do many trials, the number of times outcome x_i occurs is proportional to $P(x_i)$.

- $P(x_i)$ is for outcomes with *discrete* results, like numbers show on a pair of dice. If experiments have *continuously distributed* outcomes, like the location x of a particle, we adopt the notation $p(x)$. Now x is a real number and $p(x)$ is the *probability density*. The likelihood of seeing any outcome x is zero! However, $p(x)dx$ is the probability of seeing x fall somewhere within x and $x + dx$. It is nonzero, in general, for finite dx.

- Some rules for probability are $P(x_i) \geq 0$ and $\Sigma_i P(x_i) = 1$ ... probabilities are positive and normalized. Normalization for $p(x)$ would be $\int p(x)dx = 1$.

- The *addition rule* of probability applies when we do an experiment with an exclusive outcome, but ask a less-exclusive question. For example, we can ask about the likelihood of an outcome being x_i *OR* x_j when the experiment is done once. The answer is:
  $Prob(x_i\ OR\ x_j) = P(x_i) + P(x_j)$.

- Another rule has to do with doing more than one trial, or doing trials of two different kinds of experiments as in B&B section 3.6 which talks about "independent random variables". The most basic question is: What is the likelihood of seeing x_i AND x_j as results of two trials. If trials are independent, the *multiplication rule* applies: $Prob(x_i\ AND\ x_j) = P(x_i)P(x_j)$.

- The *mean* or *average* of a probability distribution is an important concept: $\bar{x} = \Sigma_i x_i P(x_i)$. For continuous distributions, it is $\bar{x} = \int x p(x)dx$.

- A related idea, is the expected value of a function, $f(x)$. If outcome x has a probability density $p(x)$, then
  $\bar{f} = \int f(x)p(x)dx$.

- The *moments* of a probability distribution are $\mu_j \equiv \overline{x^j}$. The first moment, μ_1 is the mean. Often, people calculate "central moments" instead: $\Delta\mu_j \equiv \overline{(x - \bar{x})^j}$. The first central moment is thus zero. The second central moment, $\Delta\mu_2$ is also known as the *variance*: $\sigma^2 = \overline{(x - \bar{x})^2}$. Its square root is, for many distributions we will encounter, a measure of the "width" of the distribution, in that most outcomes fall within $\pm\sigma$ of the mean, $\bar{x}$.

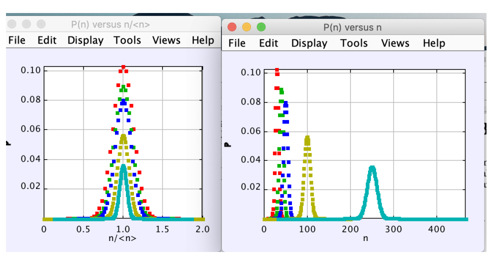
- Having more than one independent random variable, finding mean or variance of a product or sum, is treated in B&B sections 3.5 and 3.6.

- A *Bernoulli process* concerns an object which can have only two states, for example, a coin showing heads or tails, but N independent objects are considered ... either by repeating the experiment with one object N times, or by examining N objects all at once. An important parameter of the distribution is p, the probability of the first outcome (heads, say) Thus $q = 1 - p$ is the probability of tails. A "fair" coin has $p = q$. The distribution $P_N(n)$ with n the number of heads among N tosses is the *Binomial distribution*.

$$P_N(n) = \frac{N!}{n!(N-n)!} p^n q^{N-n}$$

  Please know how to calculate its mean, Np, and variance, Npq, and note that the entries of *Pascal's triangle* correspond to the values $P_N(n)$.

- Below is a graph of $P_N(n)$ from the G&T Binomial applet for increasingly larger values of N: If you look at an early version of this applet,

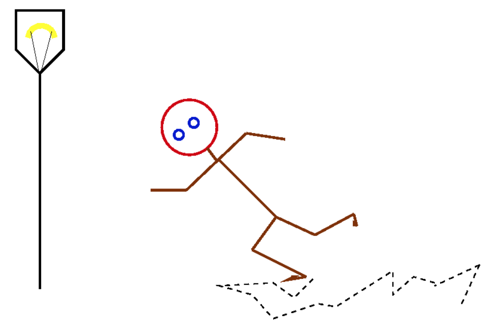


  still visible at http://stp.clarku.edu/simulations/binomial/index.html, you will see that for $N > 20$, G&T used *Stirling's approximation* for $N!$:

$$lnN! \approx NlnN - N + \frac{1}{2} ln(2\pi N)$$

  We often need $N!$ for very large N values, so please get comfortable with Stirling's approximation, derived in Appendix C.3 of B&B.

- Another Bernoulli process is the *random walk*. Random walks in space (shape of polymers) and time (paths of photons in the stellar interior) show up a lot in physics!



- Mathematical functions and integrals everyone should know:
  - The factorial integral (in Appendix C.1 of B&B)
  - The gaussian integrals (in Appendix C.2 of B&B)
  - The combination (or binomial coefficient) $C(n,r) \equiv \begin{pmatrix} n \\ r \end{pmatrix} \equiv \frac{n!}{(n-r)!\ r!}$

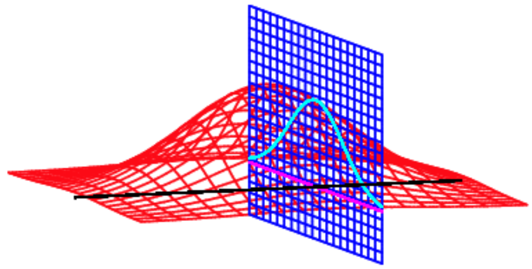
- Trials of an experiment yield *samples* for a histogram. You can estimate the moments of the true, underlying probability distribution from the histogram. The *law of large numbers* says that the more trials you do, the closer the mean, variance, ... will come to the one predicted by the true distribution.

- Suppose you find the *sum* of the results of a set of trials: $S = \Sigma_i^N s_i$. Even if $p(s_i)$ is not a Gaussian distribution, $p(S)$ approaches a *Gaussian* as you sum an arbitrarily large number, N, of results. This is the *Central Limit Theorem.*

$$p(S) = \frac{1}{\sqrt{2\pi\sigma_S^2}}\ exp[-(S-\bar{S})^2/2\sigma_S^2] \quad ; \quad \bar{S} = N\bar{s}\ ; \quad \sigma_S^2 = N\sigma^2$$

- How can we quantify ignorance? G&T section 3.4.1 says that *uncertainty* in a system with probabilities $\{P_i\}$ can be characterized by a function $S(\{P_i\})$. In order for uncertainties for subsystems to be additive, $S = -\Sigma_i P_i ln(P_i)$. In the special case that $P_i = 1/\Omega$ for all i, one has $S = ln\Omega$.

- Normalization is a *constraint* on the function $p(x)$. The method of *Lagrange's undetermined multipliers* is a clever way to maximize a function subject to a constraint like this. (It also works for multiple constraints ... we'll exploit this next week.)



- The normalization constraint on $p(x)$ is a simple idea with huge physical consequences. S subject to this constraint implies that all states are equally probable. This is discussed in the Pratt reading. (Next week, a second constraint is applied: the mean of the energy is known. This will lead us to the *Boltzmann distribution* of states: $P_j \propto e^{-\beta E_J}$.)

- G&T Ch. 4.1 begins to outlines the methods of stat mech:

  - Specify macrostates and the microstates that contribute to each macrostate.
  - Choose the *ensemble*. This is a collection of identically-prepared systems, like the different trials from probability theory. For example, if energy is the same for all members, this is called the *microcanonical ensemble*
  - Calculate statistical properties.

- Section 4.1 of G&T has a classic example: distinguishable particles with *two spin states* (identical statistics to the atoms of Section 1.4 in B&B). (Next week we'll read Section 4.2 and consider another classic example: the *Einstein solid*.)