Physics 170:
Statistical Mechanics and Thermodynamics

Lecture 1A

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Brief History

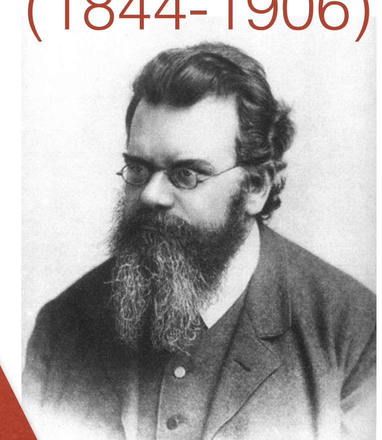
Thermodynamics

Carnot (1796-1832)

Reflections on the Motive Power of Fire

Statistical Mechanics

Boltzmann (1844-1906)

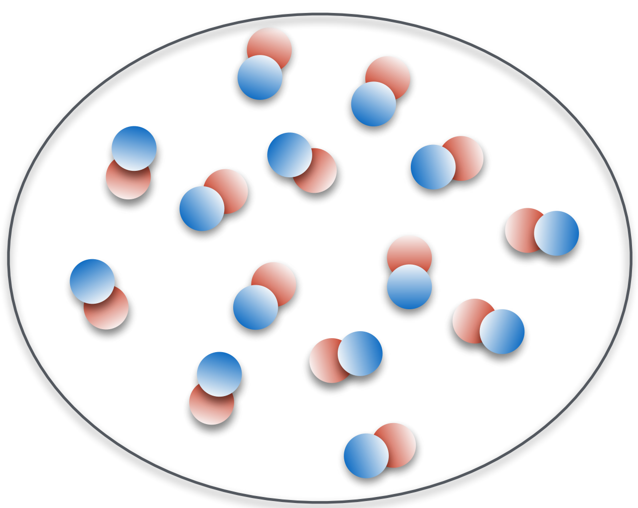


Kinetic theory of gases

Statistical Mechanics

Microscopic description

Macroscopic properties



- Quantum mechanics
- Mechanics
- E&M

E.g.:
Temperature
Pressure
Entropy
Magnetization

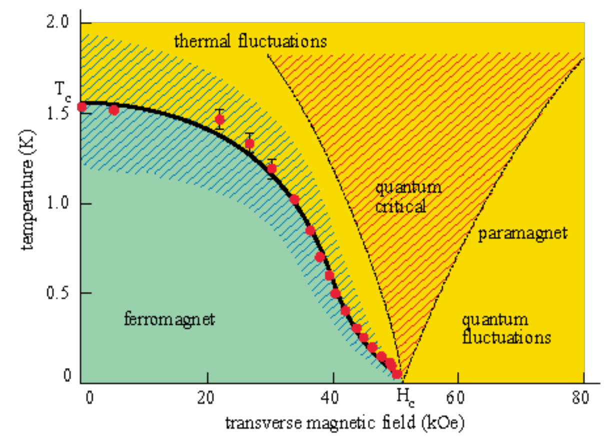
Response functions:

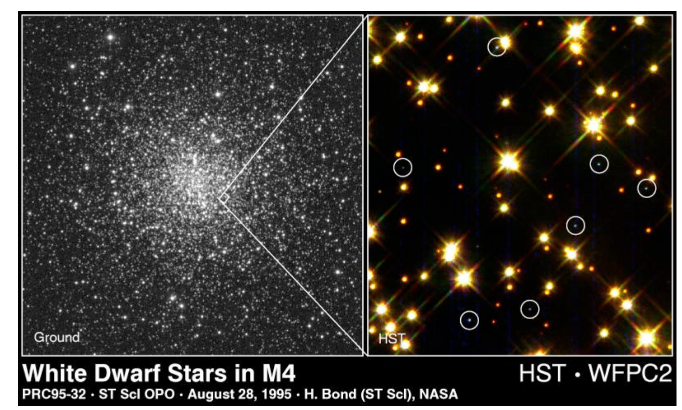
- Heat capacity
- Compressibility
- Magnetic susceptibility

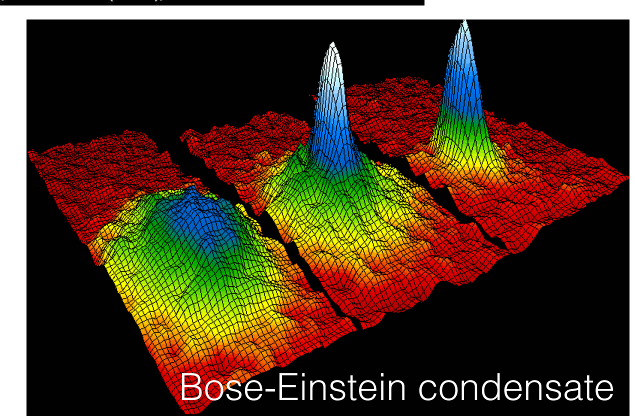
+ phase transitions, etc.

Physics 170 (+171)

Thermodynamics







etc.

Statistical Mechanics

Course Schedule

- **Lectures:** (M)/W/F 1:30 - 2:50 pm
  - Monday will *usually* be section held by TAs
  - You are responsible for material covered in section
- **Course staff**
  - Quinn MacPherson (TA)
  - Chris Overstreet (TA)
  - Ryan Hazelton (Physics Education Fellow)
- **Problem sets:** due Tuesday in Hewlett mailboxes
- **My office hour:** Monday 11-12 + by appointment

Course Information

Textbook: Kittel & Kroemer, *Thermal Physics*

Supplements:

- Reif, *Fundamentals of Statistical and Thermal Physics*
  …will be required for Physics 171.
- Notes on *Canvas* (including Prof. Kapitulnik's)

Grading:

- Problem sets (40%)
- Midterm (20%)
- Final exam (30%)
- In-class exercises (10%)

Active Learning

- Each class is structured around a **worksheet**
  (*vs.* me lecturing for 80 minutes & you falling asleep)

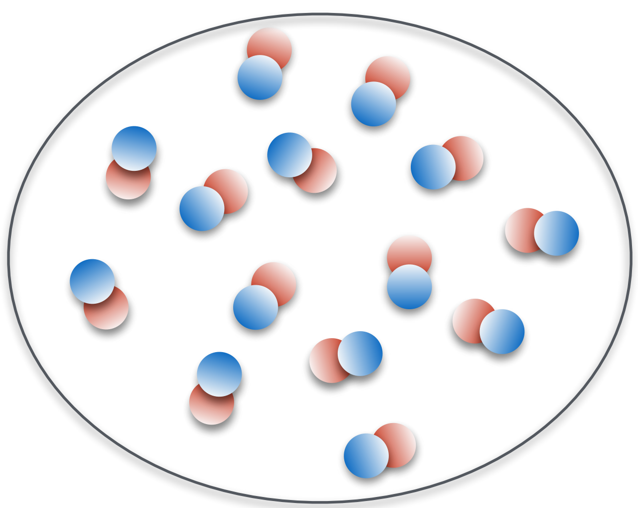
- **You are encouraged to work in groups of 3.**
  Start by choosing a scribe who has the "official" version, which I will sometimes collect at end of class.

- I always post **lecture notes, including filled out worksheet,** on Canvas after class.

- I will also announce recommended reading in advance, for those who like to see the material before class.
  For Friday: Chapter 1 of Kittel and Kroemer.

Statistical Mechanics

Microscopic description $\xrightarrow{?}$ Macroscopic properties



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+ phase transitions, etc.

* Introductions

  Chris Overstreet

  Quinn MacPherson

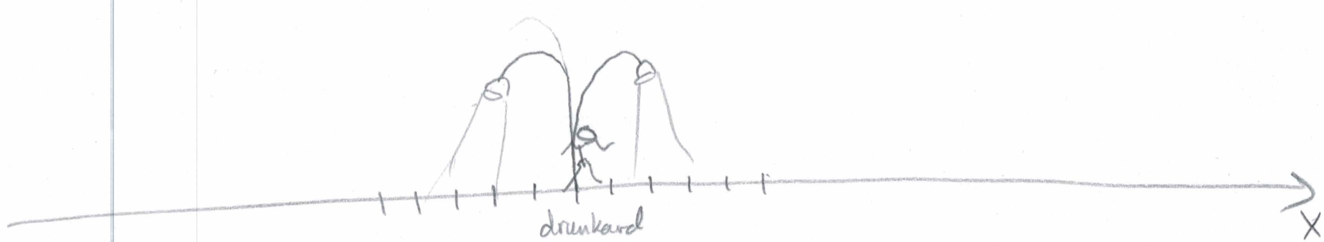
  Ryan Hazelton — Ph.D. in physics education research

  We are interested understanding what concepts are hardest to grasp in learning stat. mech. & finding ways of assessing what works in teaching them

* What is statistical mechanics?

* Course Information

* The Random Walk



N steps, each left or right ... Probabilities p, $q = 1 - p$

p ← right, q ← left

Probability distribution $P_N(X)$ for where he ends up?

Names:

EXERCISE 1A: RANDOM WALK

Objectives:

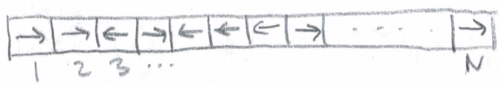
- Derive the binomial distribution describing the statistics of a random walk
- Calculate and visualize the mean and variance of the binomial distribution

Reference: Kittel & Kroemer, Ch. 1

1. A drunkard, initially standing under a lamppost, sets out on a random walk along a road, taking either a step to the right with probability p or a step to the left with probability $q = 1 - p$.

   a. After a total of N steps, what is the probability $P_N(X)$ to find the drunkard a distance of X steps to the right of the lamppost ($-N \leq X \leq N$)? Derive your answer based on the following considerations:

      i. How many different sequences of N steps are possible?



2^N sequences

      ii. How many of these sequences include R steps to the right (and $N - R$ steps to the left)? Explain your reasoning. (Extra: prove!)

As suggested by the diagram above, the problem is equivalent to asking for the # of different ways of putting R right arrows into N boxes:

$$\frac{N(N-1)(N-2)\cdots(N-R+1)}{R!} = \frac{N!}{(N-R)!\,R!} = \binom{N}{R}$$

b/c all →'s are identical

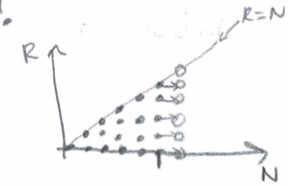
"N choose R"

* We can prove this rigourously by induction (see attached notes...) or algebraically (on homework).

* For the algebraic approach: where does $\binom{N}{R}$ show up?

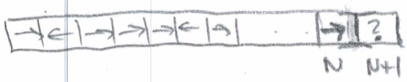
$$(a+b)^N = \sum_{R=0}^{N} \binom{N}{R} a^R b^{N-R}$$

② Inductive proof of the # of combinations $\binom{N}{R} \stackrel{?}{=} \dfrac{N!}{(N-R)!\,R!}$



* Suppose our formula is valid for some N $\forall\, R \le N$

Is it also valid for $N+1$?



$$\binom{N+1}{R} = \overset{? = \leftarrow}{\binom{N}{R}} + \overset{? = \rightarrow}{\binom{N}{R-1}} = \frac{N!}{(N-R)!\,R!} + \frac{N!}{(N-R+1)!\,(R-1)!} = \frac{N!\,[(N-R+1)+R]}{(N-R+1)!\,R!}$$

$$= \frac{(N+1)!}{[(N+1)-R]!\,R!} \quad \checkmark$$

Also: $\binom{N}{N} = \dfrac{N!}{0!\,N!} = 1 \quad \forall N \quad \checkmark$

Base case: $\binom{1}{1} = 1 \quad \checkmark$

$\therefore$ valid $\forall\, N, R$

iii. What is the probability of executing a specific one of the sequences in ii.?

$$p^R q^{N-R} = p^R(1-p)^{N-R}$$

iv. What is the probability $P_N(R)$ for the drunkard to take R steps to the right?

$$P_N(R) = \binom{N}{R} p^R (1-p)^{N-R} \xrightarrow[p=1/2]{} \frac{1}{2^N}\binom{N}{R} \checkmark$$

v. Verify that the distribution $P_N(R)$ is properly normalized.

$$\sum_{R=0}^{N} P_N(R) = \sum_{R=0}^{N} \binom{N}{R} p^R(1-p)^{N-R} \xrightarrow[\text{binomial theorem}]{} = \underbrace{[p+(1-p)]^N}_{\substack{\parallel \\ 1}} = 1$$

vi. What is the probability $P_N(X)$ for the drunkard to end up a distance X from the lamppost? Write out explicitly including factorials.

$X = R - L = R-(N-R)$
$= 2R - N \Longrightarrow R = \frac{N+X}{2}$

$$P_N(X) = \binom{N}{\frac{N+X}{2}} p^{\frac{N+X}{2}} (1-p)^{\frac{N-X}{2}} = \frac{N!}{\left(\frac{N+X}{2}\right)!\left(\frac{N-X}{2}\right)!} p^{\frac{N+X}{2}} (1-p)^{\frac{N-X}{2}} \quad (*)$$

This is a bit messy... to get an intuition for how $P_N(X)$ looks, let's calculate the <u>mean</u> and <u>variance</u>.

$*$ Looks reasonable, e.g. symmetric under $X \leftrightarrow -X$ and $p \leftrightarrow 1-p$.

b. Find the *mean* $\langle X \rangle$ and *standard deviation* ΔX of the drunkard's final position:

i. Write down generic expressions for the mean $\langle Y \rangle$ and second moment $\langle Y^2 \rangle$ of a random variable Y described by a discrete probability distribution $P(Y)$.

$$\langle Y \rangle = \sum_Y P(Y) \cdot Y$$

$$\langle Y^2 \rangle = \sum_Y P(Y) \cdot Y^2$$

Above assumes $\sum_Y P(Y) = 1 \Leftarrow$ properly normalized.

(What would you do otherwise?)

ii. How would you obtain the standard deviation ΔY from $\langle Y \rangle$ and $\langle Y^2 \rangle$?

$$\Delta Y = \sqrt{\langle (Y - \langle Y \rangle)^2 \rangle}$$ root-mean-square deviation from mean

$$= \sqrt{\langle Y^2 - 2Y\langle Y \rangle + \langle Y \rangle^2 \rangle}$$

$$= \sqrt{\langle Y^2 \rangle - 2\langle Y \rangle^2 + \langle Y \rangle^2}$$

$$= \sqrt{\langle Y^2 \rangle - \langle Y \rangle^2}$$

iii. For the case of the random walk, it will be convenient first to calculate the mean $\langle R \rangle$ and variance ΔR of the number of steps to the right. How are these quantities related to $\langle X \rangle$ and ΔX?

$X = 2R - N \implies \langle X \rangle = 2\langle R \rangle - N$

$\Delta X = 2\Delta R$ (at fixed N, i.e. $\Delta N = 0$)

iv. Calculate the average number of steps $\langle R \rangle$ taken to the right using $P_N(R)$.

Setup: $\langle R \rangle = \sum_{R=0}^{N} P_N(R) \cdot R = \sum_{R=0}^{N} \binom{N}{R} p^R q^{N-R} \cdot R$ where $q = 1-p$

Algebraic trick: we know that, generically, $\sum_{R=0}^{N} \binom{N}{R} p^R q^{N-R} = (p+q)^N$ $(\forall p, q)$

Let's pull down a factor of R by taking a derivative:

$$\frac{\partial}{\partial p} \sum_{R=0}^{N} \binom{N}{R} p^R q^{N-R} = \sum_{R=0}^{N} \binom{N}{R} \cdot \underline{R} p^{R-1} \cdot q^{N-R}$$

$$\Rightarrow \langle R \rangle = p \frac{\partial}{\partial p} \sum_{R=0}^{N} \binom{N}{R} p^R q^{N-R}$$

$$= p \frac{\partial}{\partial p} \left[(p+q)^N \right] = pN(p+q)^{N-1} \xrightarrow[q=1-p]{} = pN$$

$\therefore \langle R \rangle = pN$ ✓

In retrospect perhaps this was obvious, but the same trick will come in handy again and again...

Names:

v. Calculate the standard deviation $\Delta R = \sqrt{\langle R^2\rangle - \langle R\rangle^2}$ of the number of steps taken to the right.

Now we also need $\langle R^2\rangle$

$$\langle R^2\rangle = \left\{\sum_{R=0}^{N} \binom{N}{R} p^R q^{N-R} \cdot R^2\right\}_{q=1-p} = \left\{p\frac{\partial}{\partial p}\left[p\frac{\partial}{\partial p}\overbrace{\sum_{R=0}^{N}\binom{N}{R}p^R q^{N-R}}^{(p+q)^N}\right]\right\}_{q=1-p}$$

$$= p\frac{\partial}{\partial p}\left[pN(p+q)^{N-1}\right]$$

$$= p\left[N(p+q)^{N-1} + pN(N-1)(p+q)^{N-2}\right]$$

$$= p\left[N + pN(N-1)\right]$$

$$\Rightarrow \langle R^2\rangle - \langle R\rangle^2 = pN + p^2N(N-1) - p^2N^2 = (p-p^2)N = Np(1-p) = \Delta R^2$$

$$\therefore \Delta R = \sqrt{Np(1-p)}$$

vi. Based on iii.-v., determine $\langle X\rangle$ and ΔX. Evaluate your results explicitly for the special cases $p = 0$, $p = 1/2$, $p = 1$. Do they make sense?

$$\langle X\rangle = 2\langle R\rangle - N = (2p-1)N$$

$$\Delta X = 2\Delta R = 2\sqrt{Np(1-p)}$$

$p=0$: $\langle X\rangle = -N$ (all steps left), $\Delta X = 0$ ✓

$p=\frac{1}{2}$: $\langle X\rangle = 0$, $\Delta X = \sqrt{N}$ ← characteristic scaling for random walk — variance $\propto N$

$p=1$: $\langle X\rangle = N$ (all steps right), $\Delta X = 0$ ✓

c. Compare the random walk of the human drunkard with a random walk undertaken by an ant, both tending towards the right with probability $p = 3/4$. The drunkard takes steps of length $\ell = 40$ cm, whereas the ant takes steps of length $\ell = 1$ mm. Each walks the same total distance $L = N\ell = 10$ m, but each with a different number of steps N. Sketch, on a single set of axes, probability distributions for the final positions $x = X\ell$ of the drunkard and the ant.

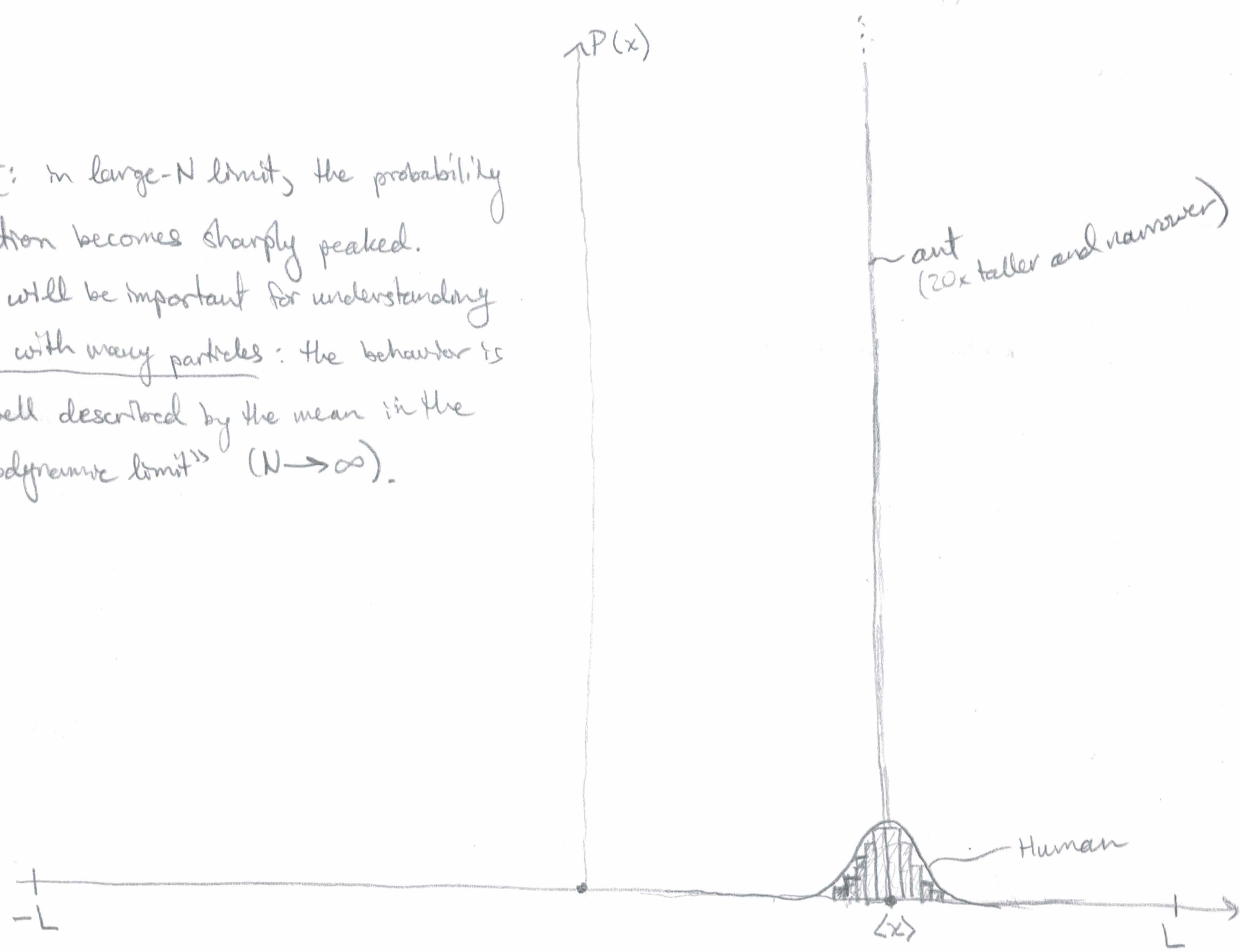
$x = \ell X = \frac{L}{N} \cdot X$

$\langle X \rangle = N(2p-1) = \frac{N}{2}$ $\qquad \Delta X = 2\sqrt{Np(1-p)} = \sqrt{3N}/2$

$\langle x \rangle = \ell \langle X \rangle = L/2$ $\qquad \Delta x = \frac{L}{2}\sqrt{3/N}$

		$\sqrt{N}$
Ant:	$N = 10^4$ steps	100
Human:	$N = 25$ steps	5

Comment: in large-N limit, the probability distribution becomes sharply peaked. This will be important for understanding systems with many particles: the behavior is very well described by the mean in the "thermodynamic limit" ($N \to \infty$).



Two other commonly encountered probability distributions arise as limiting cases of the binomial distribution. The limit $p \ll 1$ yields the *Poisson distribution* (the "law of rare events"), which you will derive in the homework. We will next consider the large-N limit, where the size of each individual step is small (i.e., ant-like) compared to the total length of the walk. This limit will lead us to the *Gaussian distribution*, and to a profound theorem that explains why we encounter the Gaussian in so many different contexts.

For next time: think of other phenomena that can be modeled as random walks...