Quantum review:

- Conjugate variables: $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \leftrightarrow \Delta x \Delta p \geq \frac{\hbar}{2}$
- $p(x) = |\psi(x)|^2$, $\int_{-\infty}^{\infty} dx |\psi(x)|^2 = P_{total} = 1$ (probability)
- Tunneling (e^- needed between nuclei for bond)
- Software (like IQmol to solve $\hat{H}\psi = E\psi$)
- quantization: ψ_n, E_n $n = 0, 1, 2 \ldots$ (n = q# for each coordinate)
- quantum interference: bond, $\psi = \psi_A + \psi_B$ antibond, $\psi = \psi_A - \psi_B$
- $\psi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2) \ldots - \psi_1(x_2)\psi_2(x_1)$ antisymmetric product, Pauli
- HOMO vs. LUMO
  - heat
  - light

Lecture 17: Statistical Mechanics:

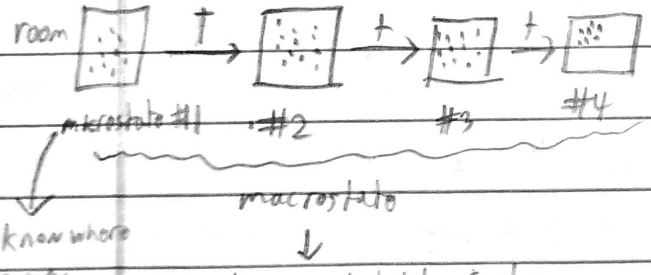
From "micro" to "macro"

Mechanics → Statistical Mechanics → Thermodynamics → Collective dynamics (micro → macro)

$F = ma$	$p(x) \approx e^{-E(x)/RT}$	$PV = nRT$	$J = c \cdot v$
$H\psi = E\psi$	$S = k_B \ln W$	$\Delta G = \Delta G^\circ + RT \ln Q$	$\langle x^2 \rangle = 6Dt$

Definitions:

- Isolated system: a collection of particles with a time-independent Hamiltonian.
- microstate vs. macrostate:



- state functions: macroscopic variables required to uniquely specify a macrostate

(in many situations, color doesn't change, won't specify a macrostate. But can in some cases)

Probability density:

ex. $|\psi|^2 = p(x)$ "probability per unit distance"

$$\int_{-\infty}^{\infty} dx\, p(x) = 1$$

ex. Probability of getting # from a die:

$$p_i = \frac{1}{6} \qquad p_{tot} = p_1 + p_2 + \ldots = \sum_{i=1}^{6} p_i = 1$$