

Newton's equation:

$$m\ddot{q} = F = -\frac{dV}{dq}$$

↳ conservative force  $\Rightarrow$  Derivative of a potential

Hamiltonian Approach:

$$H(p, q) = p\dot{q} - L(\dot{q}, q)$$

↳

$$\frac{\partial H}{\partial p} = \dot{q} \quad \frac{\partial H}{\partial q} = -\dot{p}$$

Hamilton's equation of motion

Lagrangian approach:

Define  $L(\dot{q}, q) \equiv K(\dot{q}) - V(q)$

$$\frac{\partial L}{\partial \dot{q}} = \frac{\partial K}{\partial \dot{q}} = m\dot{q}$$

$$\frac{\partial L}{\partial q} = -\frac{\partial V}{\partial q}$$

Thus,

$$\boxed{\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q}}$$

$m\ddot{q} = F$

Newton's equation in terms of Lagrangian

# Thermodynamics:

Work done by the system

$$W = \int_A^B P dV$$

Heat absorbed by the system

$$Q = \int_A^B dq$$

$$\underbrace{Q - W}_{\text{path functions}} = \underbrace{\Delta E}_{\text{State fn}} \rightarrow \text{Change in internal energy}$$

→ First law of thermodynamics

Change in entropy

$$\Delta S = \int_A^B \frac{dq_{\text{rev}}}{T}$$

for a reversible process

Second law

for all other processes

$$\Delta S > \int_A^B \frac{dq}{T} \Rightarrow$$

$$\boxed{ds > \frac{dq}{T}}$$

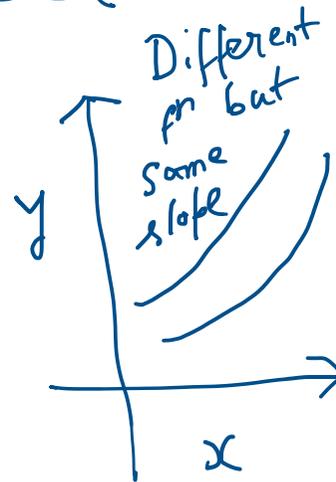
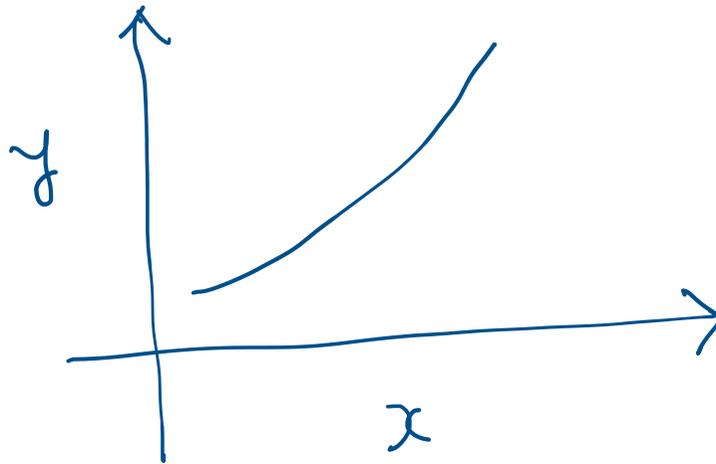
$$S - S_0 = \int_0^T \frac{dq_{rev}}{T} = S \quad \text{as } S_0 = 0 \quad (\text{S at } T=0 \text{ is zero})$$

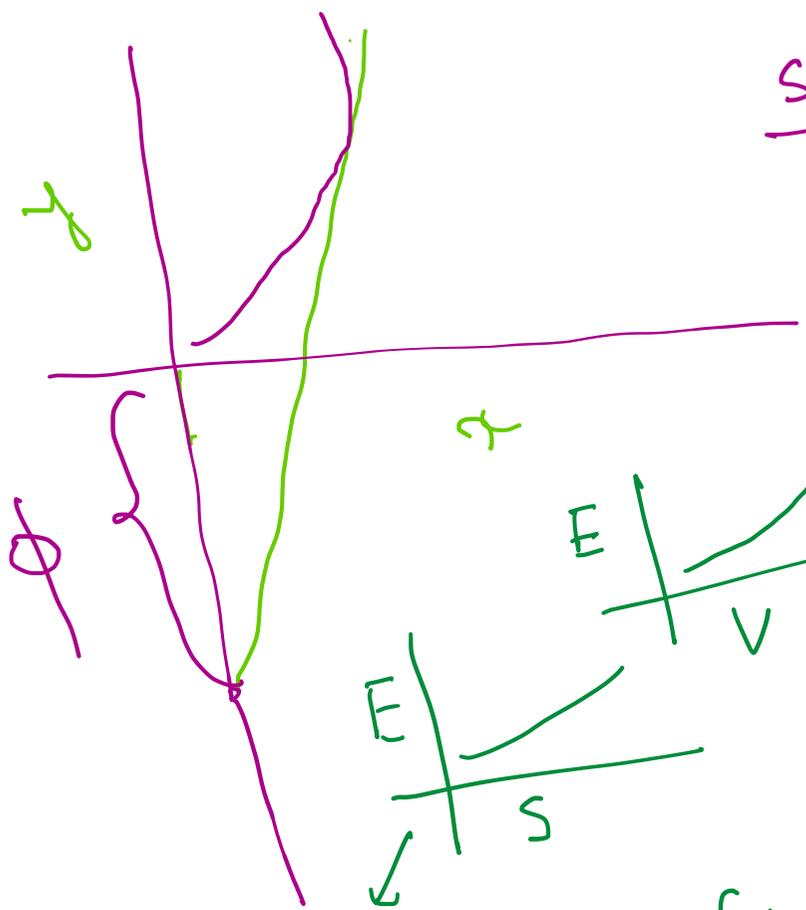
"third law"

$$dE = dq - dw \quad \text{First law}$$

$$dE = T ds - P \cdot dv \rightsquigarrow (S, V) \text{ are the natural variables for } E \equiv E(S, V)$$

$$\left( \frac{\partial E}{\partial S} \right)_V = T \quad \left( \frac{\partial E}{\partial V} \right)_S = -P$$





Slope:

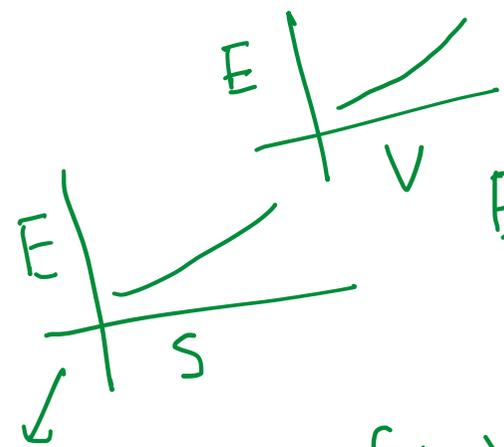
$$p = \frac{y - \phi}{x - 0} \Rightarrow$$

Slope  
(not pressure or momentum)

$$\phi(p) = y - px$$

$$y(x) \Leftrightarrow \phi(p = \frac{dy}{dx})$$

Legendre transformation



$$E(S, V) \Rightarrow f(T, V)$$

$$E(S) \Rightarrow f(T)$$

$$f(T) = E - TS = A(T, V)$$

→ Helmholtz free

$$dE = TdS - P \cdot dV$$

$$\left(\frac{\partial E}{\partial S}\right)_V = T; \left(\frac{\partial E}{\partial V}\right)_S = -P$$

$$g = E - \left(\frac{\partial E}{\partial V}\right)_S V = E + PV \rightarrow \text{enthalpy}$$

$$H(p, q) = p\dot{q} - L(\dot{q}, q)$$

$$H(p) = p\dot{q} - L(\dot{q})$$

$$f(p) = L(\dot{q}) - \left(\frac{\partial L}{\partial \dot{q}}\right) \dot{q}$$

$$f(p) = L(\dot{q}) - p\dot{q}$$

$$-f(p) = p\dot{q} - L(\dot{q})$$

$$\xrightarrow{\quad} H(p)$$

$$\phi(p) = y - px$$

Not momentum  
 $p = \frac{dy}{dx}$

$$\frac{\partial L}{\partial \dot{q}} = p$$

→ They are related by Legendre transformations

# Quantum Mechanics:

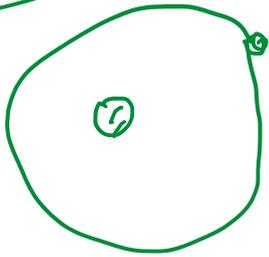
Probabilistic

$$\psi(x, t) \quad \psi(q, t)$$

$$\int dx \psi^*(x, t) \psi(x, t) \rightarrow \text{Probability density}$$

↓  
Total probability

H-atom

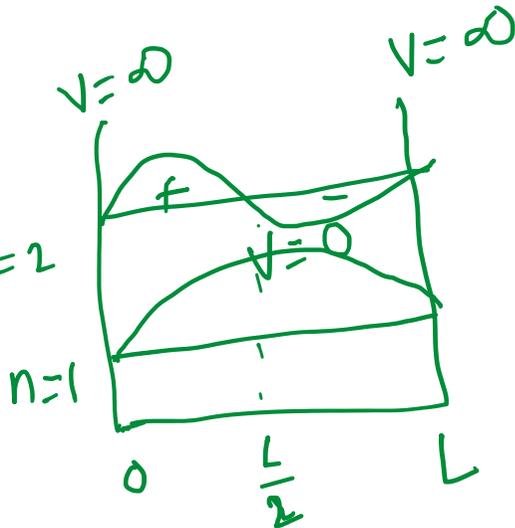


Simple Harmonic Oscillator  
(SHO)

Rigid Rotors

Particle in a box:  $n=2$

$$E = \frac{n^2 h^2}{8mL^2}$$



Time independent

Schrodinger's equation

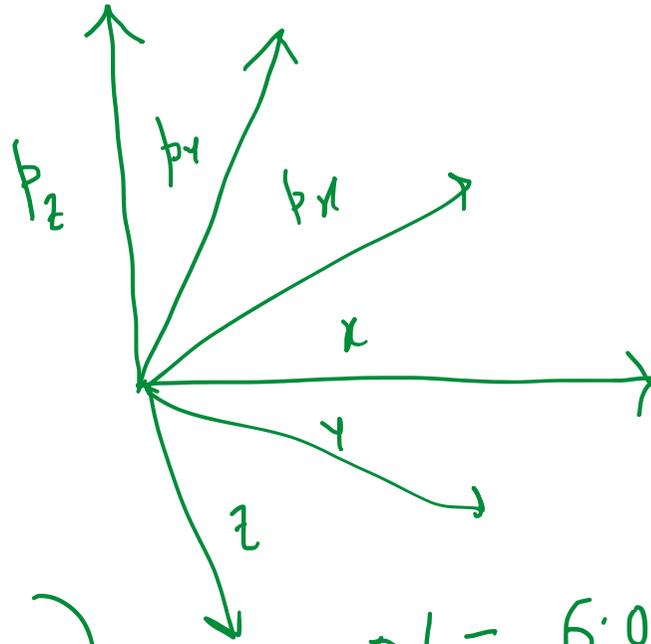
$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi$$

$$\hookrightarrow \psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Single particle

## Phase Space

$(q, p)$   
↓  
 $x, y, z$   
↘  
 $p_x, p_y, p_z$   
6-co-ordinates



Think of N particles

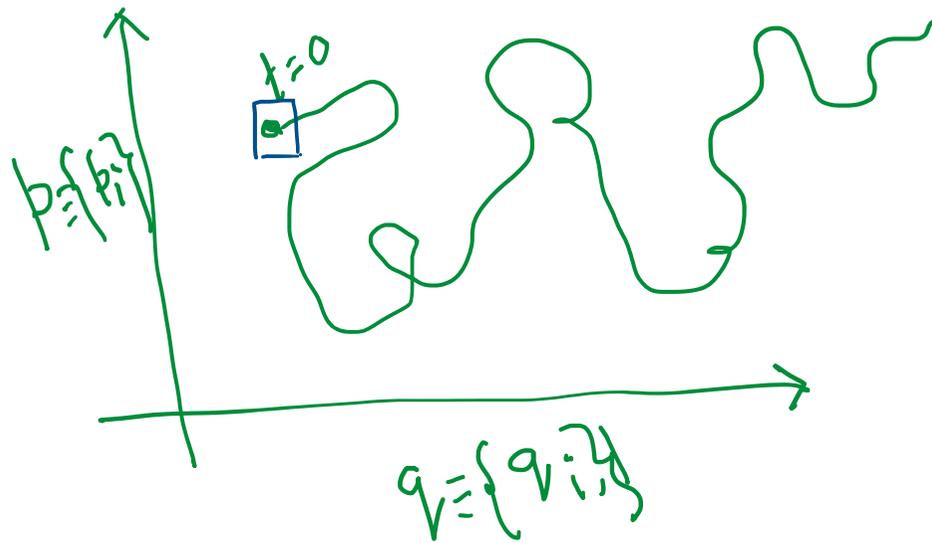
$3N \rightarrow$  position  
co-ordinates

$3N \rightarrow$  momentum  
co-ordinates

$$N = 6.023 \times 10^{23}$$
$$6N = 36 \dots \times 10^{23}$$

of some given Huge No.  
time

$\{p_i, q_i\}$  or  $\{q_i, p_i\} \Rightarrow$  phase space  $\rightarrow 6N$  dimensional



Phase Space trajectory

What is rule the system follows in this phase space?

Each of these particles is following Newton's equation

No Computer in this world can store

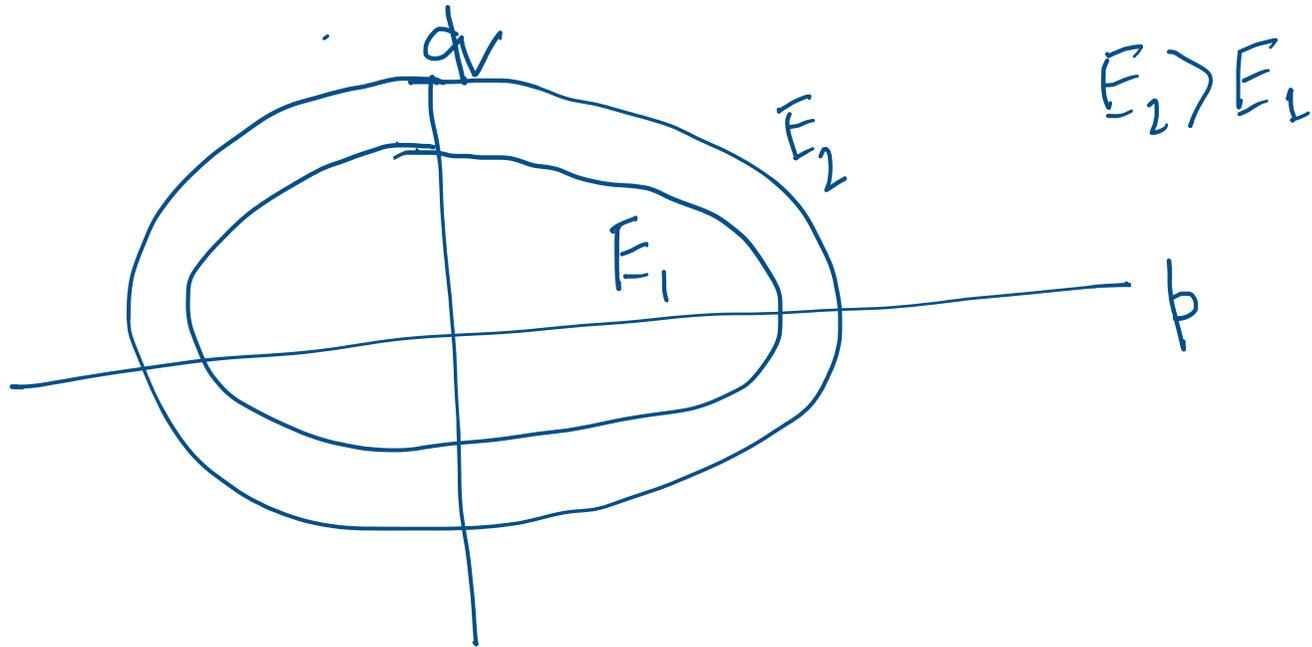
$\rightarrow$  Phase space distribution  $f^n \rightarrow f(p_i, q_i, t)$

$\rightarrow$  follows some eq<sup>n</sup>  $\rightarrow$  Liouville's eq<sup>n</sup>

# Simple Harmonic Oscillator

SHO

$$H = \frac{p^2}{2m} + \frac{1}{2}kq^2 = E_{\text{Total}}$$

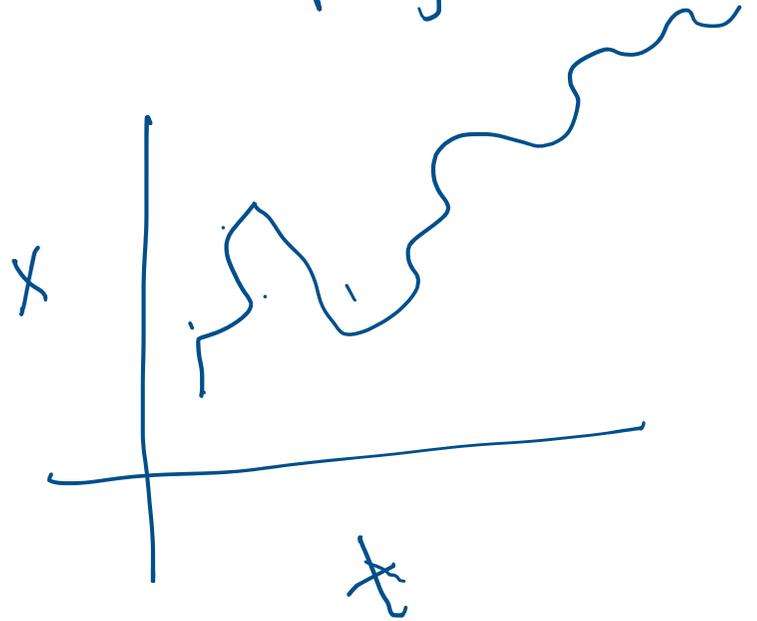


Time Average:

$$\bar{X} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_{t_0}^{t_0 + \tau} ds X(s)$$

→ time average  
over a  
long  
trajectory

$$\bar{X} = \lim_{t \rightarrow \infty} \frac{1}{t} \int_{t_0}^{t_0 + t} dt' X(t')$$



# Ensemble & Ensemble average:

Microstate of a system  $\rightarrow (p_i, q_i)$

Macrostate  $\Rightarrow$  Many microstates  
 can correspond  
 to a single macrostate

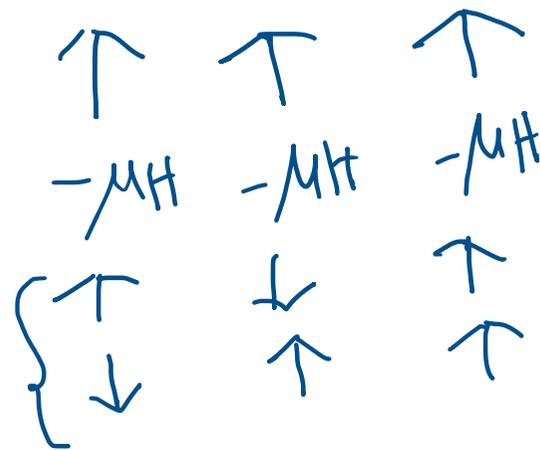


Magnetic system (three tiny magnets)

External magnetic field

$$E = -\vec{\mu} \cdot \vec{H}$$

two microstates



$$E = -3\mu H$$

$$\left. \begin{array}{l} E = -\mu H \\ E = -\mu H \end{array} \right\} \text{Same macrostate}$$