

# Quantum Mechanics

03 October 2011

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## Evaluation

2 mid term exams - 20% of final grade

One final - 80% of final grade

# Schrodinger eq

03 October 2011

14:09

Qm- 1900

Schrodinger- 1925

Eq for a function- Wavefunction  $\psi(x, y, z, t)$

Eq in partial derivatives [differential of]

For a particle of mass  $m$  under the influence of a potential  $V_x$

$$-\frac{\hbar^2}{2m} \frac{\delta^2}{\delta x^2} \psi(x, t) + V_x \psi(x, t) = i\hbar \frac{\delta}{\delta t} \psi(x, t)$$

Suppose that

$$\psi(x, t) = e^{-\frac{iE}{\hbar}t} \psi(x)$$

(stationary state)

And put it in schrodinger eq

$$\frac{\delta}{\delta t} \psi(x, t) = -\frac{i}{\hbar} E e^{-\frac{iE}{\hbar}t} \psi(x)$$

$$i\hbar \frac{\delta}{\delta t} \psi(x, t) = E e^{-\frac{iE}{\hbar}t} \psi(x)$$

$$\frac{\delta^2}{\delta x^2} \psi(x, t) = \frac{\hbar}{m} e^{-\frac{iE}{\hbar}t} \psi''(x)$$

$$V\psi = e^{-\frac{iE}{\hbar}t} v\psi(x)$$

$$-\frac{\hbar^2}{2m} \psi'' + V(x)\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m} \psi'' + (V - E)\psi = 0$$

$$\psi(x, t) = A e^{-\frac{iE}{\hbar}t} e^{-\lambda x^2}$$

1)  $i\hbar \frac{\delta}{\delta t} \psi(x, t)$

2)  $\frac{\delta \psi}{\delta x}$

3)  $-\frac{\hbar^2}{2m} \frac{\delta^2 \psi}{\delta x^2}$

1)  $AE A e^{-\frac{iE}{\hbar}t} e^{-\lambda x^2}$

2)  $A e^{-\frac{iE}{\hbar}t} (-2\lambda x) e^{-\lambda x^2}$

3)  $\frac{\hbar^2}{2m} A e^{-\frac{iE}{\hbar}t} 2\lambda(2\lambda x^2 e^{-\lambda x^2} - e^{-\lambda x^2})$

$$-\frac{\hbar^2}{2m} A e^{-\frac{iE}{\hbar}t} e^{-\lambda x^2} (4\lambda^2 x^2 - 2\lambda) + V A e^{-\frac{iE}{\hbar}t} e^{-\lambda x^2} = AE e^{-\frac{iE}{\hbar}t} e^{-\lambda x^2}$$

$$-\frac{\hbar^2}{2m} (4\lambda^2 x^2 - 2\lambda) + V_x - E = 0$$

$$V = \alpha_1 x^2 + \alpha_2$$

$\psi(x, t)$  is the wavefunction of a system

$\psi^*(x, t) \times \psi(x, t) = |\psi(x)|^2 \rightarrow$  probability of the system to be between  $(x, x+dx)$

What we need to impose on a wavefunction?

1. Solves schrodinger eq

$$-\frac{\hbar^2}{2m} \frac{\delta^2}{\delta x^2} \psi(x, t) + V_x \psi(x, t) = i\hbar \frac{\delta}{\delta x} \psi(x, t)$$

2. It has to be differentiable

3. Simple valued

4. Normalizable  $\int_{-\infty}^{\infty} dx |\psi(x)|^2 = 1$

$$\psi(x, t) = A e^{-\frac{iE}{\hbar}t} e^{-\lambda x^2}$$

For a particular  $V(x) \rightarrow$  solve schrodinger eq

$$\psi\psi^* = |A|^2 e^{-2\lambda x^2}$$

$$|A|^2 \int_{-\infty}^{\infty} e^{-2\lambda x^2} dx = |A|^2 \sqrt{\frac{\pi}{2\lambda}}$$

$$\int_{-\infty}^{\infty} e^{-\lambda x^2} dx = \sqrt{\frac{\pi}{\lambda}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\lambda x^2} dx = \sqrt{\frac{\pi}{2\lambda^3}}$$

$$\psi(x, t) = A e^{-\frac{iE}{\hbar}t} e^{-\lambda x^2}$$

For a particular  $V(x) \rightarrow$  solve schrodinger eq

$$\psi\psi^* = |A|^2 e^{-2\lambda x^2}$$

$$|A|^2 \int_{-\infty}^{\infty} e^{-2\lambda x^2} dx = |A|^2 \sqrt{\frac{\pi}{2\lambda}}$$

$$\Psi(x, t) = e^{-\frac{i}{\hbar}Et} \psi(x)$$

Stationary states

$$-\frac{\hbar^2}{2m} \psi''(x) + V(x)\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m} \psi'' + (V - E)\psi = 0$$

Useful today

$$\int_{-\infty}^{\infty} e^{-\sigma x^2} dx = \sqrt{\frac{\pi}{\sigma}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\sigma x^2} dx = \sqrt{\frac{\pi}{4\sigma^3}}$$

$$\int_{-\infty}^{\infty} x e^{-x^2} dx = 0$$

1. Continuous, differentiable
2. Normalizable

$$\int_{-\infty}^{\infty} dx \psi(x, t) \psi^*(x, t) = \int_{-\infty}^{\infty} dx |\psi|^2 = 1$$

$$\psi(x, t) = A e^{-\frac{i}{\hbar}Et} e^{-\lambda x^2}$$

Plug this in to the schrodinger eq to find a solution  $\rightarrow V \sim (x^2 + p)$

$\lambda$  positive real number

A Some number

$$|\psi|^2 = |A|^2 e^{-2\lambda x^2}$$

Calculate

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) x \psi(x, t) dx = \left(\frac{2\lambda}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-2\lambda x^2} x dx = 0$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* x^2 \psi = \left(\frac{2\lambda}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-2\lambda x^2} x^2 dx = \left(\frac{2\lambda}{\pi}\right)^{\frac{1}{2}} \sqrt{\frac{\pi}{4 * 8\lambda^3}} = \sqrt{\frac{1}{16\lambda^2}}$$

$$(\Delta x) = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{1}{4\lambda}}$$

$$f(x) = e^{-\sigma x^2}$$

$$f' = -2\sigma x e^{-\sigma x^2}$$

$$f'' = (-2\sigma + 4\sigma^2 x^2) e^{-\sigma x^2}$$

Useful today

$$\int_{-\infty}^{\infty} e^{-\sigma x^2} dx = \sqrt{\frac{\pi}{\sigma}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\sigma x^2} dx = \sqrt{\frac{\pi}{4\sigma^3}}$$

$$\int_{-\infty}^{\infty} x^{2m+1} e^{-\sigma x^2} dx = 0$$

$$\psi(x, t) = \left(\frac{2\lambda}{\pi}\right)^{\frac{1}{4}} e^{-\frac{i}{\hbar}Et} e^{-\lambda x^2}$$

$$1. |\psi|^2 = |A|^2 e^{-2\lambda x^2} \rightarrow \text{imposed} \rightarrow \int_{-\infty}^{\infty} |\psi|^2 dx = 1 \rightarrow A = \left(\frac{2\lambda}{\pi}\right)^{\frac{1}{4}}$$

$$2. \langle x \rangle = 0 = \int_{-\infty}^{\infty} \psi^* x \psi dx = |A|^2 \int_{-\infty}^{\infty} x e^{-2\lambda x^2} dx = 0$$

$$3. \langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* x^2 \psi dx = |A|^2 \int_{-\infty}^{\infty} e^{-2\lambda x^2} x^2 dx = \frac{1}{4\lambda}$$

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{2\sqrt{\lambda}}$$

$$\lambda \rightarrow \infty, \Delta x \rightarrow 0$$

$$\lambda \rightarrow 0, \Delta x \rightarrow \infty$$

Define

Momentum operator

$$p = \frac{\hbar}{i} \frac{\delta}{\delta x}$$

$$\nabla f = \frac{\delta f}{\delta x} i + \frac{\delta f}{\delta y} j$$

$$p\psi(x, t) = \frac{\hbar}{i} \frac{\delta}{\delta x} \psi(x, t)$$

$$p^2\psi(x, t) = pp\psi$$

$$\frac{\hbar}{i} \frac{\delta}{\delta x} \left( \frac{\hbar}{i} \frac{\delta}{\delta x} \psi \right) = -\hbar^2 \frac{\delta^2}{\delta x^2} \psi$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \left( \frac{\hbar}{i} \right) \frac{\delta}{\delta x} \psi dx = \int_{-\infty}^{\infty} \frac{\hbar}{i} \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{2}} (-2\lambda x) e^{-2\lambda x^2} dx = \frac{\hbar}{i} \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} (-2\lambda x) e^{-2\lambda x^2} dx$$

$$= \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{2}} \frac{\hbar}{i} (-2\lambda) \int_{-\infty}^{\infty} x e^{-2\lambda x^2} dx = 0$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \psi^* (-\hbar^2) \frac{\delta^2}{\delta x^2} \psi dx = \int_{-\infty}^{\infty} \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{4}} e^{\frac{1}{\hbar} Et} e^{-\lambda x^2} (-\hbar^2) \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{4}} e^{-\frac{1}{\hbar} Et} (-2\lambda + 4\lambda^2 x^2) e^{-\lambda x^2} dx$$

$$= \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{4}} \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{4}} (-\hbar^2) \int_{-\infty}^{\infty} (-2\lambda + 4\lambda^2 x^2) e^{-2\lambda x^2} dx = -\hbar^2 \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} (-2\lambda + 4\lambda^2 x^2) e^{-2\lambda x^2} dx$$

$$= -\hbar^2 \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{2}} \left[ -2\lambda \sqrt{\frac{\pi}{2\lambda}} + 4\lambda \sqrt{\frac{\pi}{4 * 8\lambda^2}} \right]$$

$$\psi(x, t) = \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{4}} e^{-\frac{i}{\hbar} Et} e^{-\lambda x^2}$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \hbar \sqrt{\lambda}$$

$$\Delta x = \frac{1}{2\sqrt{\lambda}}$$

$$\Delta p = \hbar \sqrt{\lambda}$$

$$\lambda \rightarrow \infty \Delta p \rightarrow \infty$$

$$\lambda \rightarrow 0 \Delta p \rightarrow 0$$

$$\Delta x \Delta p \sim \frac{\hbar}{2}$$

Uncertainty principle

$$x = x_0 + v_0 t + \frac{at^2}{2}$$

$$f = A \cos \omega x + B \sin \omega x$$

$$f'' = -A\omega^2 \cos \omega x - B\omega^2 \sin \omega x$$

$$f'' + \omega^2 f = 0$$

Oscillator

$$f(x) = A \cos \omega x + B \sin \omega x$$

$$f(x=0) = 0 \rightarrow A * 1 + B * 0 = 0 \Rightarrow \boxed{A=0}$$

$$f(x=L) = 0 \rightarrow B \sin \omega L = 0 \left\{ \begin{array}{l} B=0 \\ \sin \omega L = 0 \end{array} \right.$$

$$\sin \omega L = 0$$

$$\omega L = k\pi$$

$$\omega = \frac{k\pi}{L}$$

$$f = B_1 \sin \left( \frac{k\pi}{L} x \right) + B_2 \sin \left( \frac{k\pi}{L} x \right)$$

$$-\frac{\hbar^2}{2m} \frac{\delta^2 \psi}{\delta x^2} + V\psi = i\hbar \frac{\delta}{\delta t} \psi$$

$$-\frac{\hbar^2}{2m} \frac{\delta^2}{\delta x^2} \psi = i\hbar \frac{\delta}{\delta t} \psi$$

$$\psi(x, t) = \psi(x) e^{-\frac{i}{\hbar} Et}$$

$$-\frac{\hbar^2}{2m} e^{-\frac{i}{\hbar} Et} \psi''(x) = i\hbar \left( -\frac{i}{\hbar} E \right) e^{-\frac{i}{\hbar} Et} \psi(x)$$

$$-\frac{\hbar^2}{2m} \psi''(x) = E\psi(x)$$

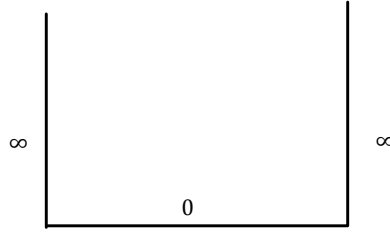
$$\psi''(x) + \omega^2 \psi(x) = 0$$

$$\omega^2 = \frac{2mE}{\hbar^2}$$



$$-\frac{\hbar^2}{2m} \frac{\delta^2}{\delta x^2} \psi + V\psi = i\hbar \frac{\delta}{\delta t} \psi$$

Last time we solved it for



Today we will study

$$V = \frac{\kappa x^2}{2}$$

As in previous lectures

Propose

$$\psi(x, t) = e^{-\frac{i}{\hbar} E t} \psi(x)$$

→ we plug this into the schrodinger eq

Check at home

$$-\frac{\hbar^2}{2m} \psi''(x) + \frac{\kappa}{2} x^2 \psi = E\psi$$

$$\psi'' + x^2 \psi = E\psi$$

$$(a^2 - b^2) = (a + b)(a - b)$$

The idea is to factorize the 2nd order eq

Define two operators

$$a_+ = \frac{1}{\sqrt{2m}} \left\{ \frac{\hbar}{i} \frac{d}{dx} + im\omega x \right\}$$

$$a_- = \frac{1}{\sqrt{2m}} \left\{ \frac{\hbar}{i} \frac{d}{dx} - im\omega x \right\}$$

$$a_+ a_- = a_+ \frac{1}{\sqrt{2m}} \left\{ \frac{\hbar}{i} \frac{d}{dx} - im\omega x \right\}$$

$$\frac{1}{\sqrt{2m}} \left\{ \frac{\hbar}{i} \frac{d}{dx} + im\omega x \right\} \frac{1}{\sqrt{2m}} \left\{ \frac{\hbar}{i} \frac{d}{dx} - im\omega x \right\}$$

$$= \frac{1}{2m} \left\{ -\hbar^2 \psi'' - \frac{\hbar}{i} im\omega \frac{d}{dx} (x\psi) + 2m\omega x \frac{\hbar}{i} \psi' + m^2 \omega^2 x^2 \psi \right\}$$

$$= \frac{1}{2m} \left\{ -\hbar^2 \psi'' - \hbar m\omega (\psi + x\psi') + m\omega \hbar x\psi + m^2 \omega^2 x^2 \psi \right\}$$

$$a_+ a_- \psi = -\frac{\hbar^2}{2m} \psi'' - \frac{\hbar\omega}{2} \psi + \frac{m\omega^2}{2} x^2 \psi$$

$$a_+ a_- \psi = E\psi - \frac{\hbar\omega}{2} \psi$$

$$\omega^2 = \frac{k}{m}$$

$$-\frac{\hbar^2}{2m} \psi'' + \frac{m\omega^2}{2} x^2 \psi = E\psi$$

$$a_- a_+ \psi = \frac{1}{\sqrt{2m}} \left\{ \frac{\hbar}{i} \frac{d}{dx} - im\omega x \right\} \frac{1}{\sqrt{2m}} \left\{ \frac{\hbar}{i} \frac{d}{dx} + im\omega x \right\}$$

$$= \frac{1}{2m} \left\{ -\hbar^2 \psi'' + \hbar m\omega (x\psi + \psi) - \hbar m\omega x\psi + m^2 \omega^2 x^2 \psi \right\}$$

$$= -\frac{\hbar^2}{2m} \psi'' + \frac{m\omega^2}{2} x^2 \psi + \frac{\hbar\omega}{2} \psi$$

$$\psi(x, t) = \sum_k c_k \sqrt{\frac{2}{L}} e^{-\frac{i}{\hbar} E_k t} \sin\left(\frac{k\pi}{L} x\right)$$

1. E quantized

$$E_k = \frac{\hbar^2 \pi^2 k^2}{2mL^2}$$

$(c_k)^2$  = probability for the particle to be in k-state

\newcommand{\~new~}{\~old~}

Summary

We study the oscillator in quantum mechanics

This means the schrodinger equation for a particlue under a potential

$$v = \frac{kx^2}{2}$$

$$\left( v = \frac{m\omega^2}{2} x^2 \right)$$

We proposed a wavefunction

$$\psi(x, t) = e^{iEt/\hbar} \psi(x)$$

We get

$$\boxed{-\frac{\hbar^2}{2m} \psi''(x) + \frac{m\omega^2}{2} x^2 \psi(x) = E\psi(x)} \quad (*)$$

Special function

Very difficult to solve

The problem here is to find

E = possible energy

$\psi(x)$  = wavefunction

Actually, there is a nice way of solving this without solving the eq (\*)

To do this we started to study an idea due to Heisenberg (st)

Last week we introduced two operators

$a_+$

$a_-$

$$[a_+, a_-] = \hbar\omega$$

$$[a_-, a_+] = \hbar\omega$$

Kinetic + potential

$$H = \frac{1}{2} mv^2 + V(x)$$

$$\frac{1}{m} mv^2 = \frac{p^2}{2m}$$

$$p = mv$$

$$\hat{p}^2 = -\hbar^2 \frac{d^2}{dx^2}$$

$$\boxed{H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)}$$

At home, show that

$$\boxed{\begin{aligned} H &= a_+ a_- + \frac{\hbar\omega}{2} \\ \text{or} \\ H &= a_- a_+ - \frac{\hbar\omega}{2} \end{aligned}}$$

We will know the result for

$$[a_+, H] = \text{show at home} - \hbar\omega a_+$$

$$[a_-, H] = \hbar\omega a_-$$

As a sample let me calculate

$$[a_-, H] = a_- H - H a_- = a_- \left( a_- a_+ - \frac{\hbar\omega}{2} \right) - \left( a_- a_+ - \frac{\hbar\omega}{2} \right) a_-$$

$$= a_- a_- a_+ - \frac{\hbar\omega}{2} a_- - a_- a_+ a_- + \frac{\hbar\omega}{2} a_-$$

$$= a_- a_- a_+ - a_- a_+ a_- =$$

$$\text{The idea is instead of } \boxed{a_- a_+ = -\hbar\omega + a_+ a_-}$$

$$a_- (-\hbar\omega + a_+ a_-) - a_- a_+ a_- = -\hbar\omega a_- + a_- a_+ a_- - a_- a_+ a_- = -\hbar\omega a_-$$

Theorem

If you have a wavefunction  $\psi_*(x)$

That solves the Schrödinger equation with energy  $E_*$

$$H\psi_* = E_*\psi_*$$

Then you can construct two other functions

$$a_+\psi_*$$

$$a_-\psi_*$$

$$\text{They will solve the Schrodinger eq } \left( \begin{array}{l} E_* + \hbar\omega \\ E_* - \hbar\omega \end{array} \right)$$

$$a_+ \rightarrow \text{satisfies the eq with } E = E_* + \hbar\omega$$

$$a_- \rightarrow \text{satisfies the eq with } E = E_* - \hbar\omega$$

$$H(a_+\psi) = [a_+, H]\psi = (a_+H + \hbar\omega a_+)\psi$$

$$= a_+E\psi + \hbar\omega a_+\psi = (E + \hbar\omega)(a_+\psi)$$

$$(a_+\psi) = \psi_+$$

$$f'(x) = ax f(x) \rightarrow \frac{1}{f(x)} \frac{df}{dx} = ax$$

$$\Rightarrow \frac{1}{f(x)} df = ax dx$$

$$\Rightarrow \int \frac{df}{f} = \int ax dx$$

$$\boxed{\log f = \frac{ax^2}{2} + c}$$

remember

$$\boxed{\int_{-\infty}^{\infty} e^{-\sigma x^2} dx = \sqrt{\frac{\pi}{\sigma}}}$$

$$f'(x) = ax f(x) \rightarrow f(x) = Ae^{\frac{ax^2}{2}}$$



$$\rightarrow f = e^c e^{-\frac{\alpha x^2}{2}}$$

$$\rightarrow f = A e^{-\frac{\alpha x^2}{2}}$$

If a wavefunction  $\psi$  with energy  $E$

$$\text{means } \boxed{H\psi = E\psi}$$

Then

$$\psi_+ = (a_+ \psi)$$

$$\psi_- = (a_- \psi)$$

Also solves the schrodinger eq but with energy

$$(E \pm \hbar\omega)$$

Energy of a particle is positive

$\psi_{\text{solution}}$

$$H\psi_{\text{solution}} = E_{\text{solution}}\psi_{\text{solution}}$$

$$a_- \psi_{\text{solution}} \rightarrow E_{\text{new}} = E_{\text{sol}} - \hbar\omega$$

$$a_- a_- \psi_{\text{sol}} \rightarrow E_{\text{new}} = E_{\text{sol}} - 3\hbar\omega$$

Since there is no negative energy, there must be some wavefunction/state such that if you apply  $a_-$

on it  $\rightarrow$  give zero

$\psi_0 =$ ground state

$$\boxed{a_- \psi_0 = 0} \rightarrow \text{solve for this } \psi_0$$

$$\frac{1}{\sqrt{2m}} \left( \frac{\hbar}{i} \frac{d}{dx} \psi_0 - im\omega x \psi_0 \right) = 0 \rightarrow \frac{\hbar}{i} \frac{d}{dx} \psi_0 = im\omega x \psi_0$$

$$\boxed{\frac{d}{dx} \psi_0 = -\frac{m\omega}{\hbar} x \psi_0}$$

$$\boxed{\psi_0 = A e^{-\frac{m\omega}{2\hbar} x^2}}$$

$$\int_{-\infty}^{\infty} \psi_0 \psi_0^* dx = |A|^2 \int e^{-\frac{m\omega}{\hbar} x^2} dx$$

Value of A is

$$A = \left( \frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}}$$

How do we calculate

$\psi_1 =$  first excited state

$$\psi_1 = a_+ \psi_0$$

$$\frac{1}{\sqrt{2m}} \left( \frac{\hbar}{i} \frac{d}{dx} \psi_0 + im\omega x \psi_0 \right) = \psi_1$$

$$\psi_1 = \frac{1}{\sqrt{2m}} \left( \frac{\hbar}{i} A e^{-\frac{m\omega}{\hbar} x^2} + im\omega x A e^{-\frac{m\omega}{\hbar} x^2} \right)$$

$$\psi_1 = \frac{1}{\sqrt{2m}} e^{-\frac{m\omega}{\hbar} x^2} (\#x)$$

If you calculate the energy of the ground state

$$H\psi_0 = \frac{\hbar\omega}{2} \psi_0$$

$$\frac{\hbar\omega}{2} = \text{energy of } \psi_0$$

$$\psi_0 = A e^{-\frac{m\omega}{\hbar} x^2}$$

$$\boxed{E_m = \left( m + \frac{1}{2} \right) \hbar\omega}$$

# Summary

07 November 2011

14:07

## Schrodinger eq

For a particle of mass  $m$  under the influence of a potential  $V(x)$  ( $f = -\frac{dV}{dx}$ )

$$-\frac{\hbar^2}{2m} \frac{\delta^2}{\delta x^2} \psi(x, t) + V(x)\psi(x, t) = i\hbar \frac{\delta}{\delta t} \psi(x, t) \rightarrow \text{you get}$$

$$-\frac{\hbar^2}{2m} \psi''(x) + V(x)\psi(x) = E\psi$$

By substituting in  $\psi(x, t) = e^{-\frac{i}{\hbar}Et}$

$$\psi = \begin{cases} \text{complex in most} \\ \text{of our examples} \\ \psi(x, t) = e^{-\frac{i}{\hbar}Et} \end{cases}$$

Wavefunction

$$\Psi(x, t) \text{ or } \psi(x) = \begin{cases} \text{differentiable} \\ \text{single valued} \\ \int_{-\infty}^{\infty} \psi\psi^* dx = 1 \rightarrow \text{"probabilities"} \end{cases}$$

$$\Psi(x, t) = e^{\frac{i}{\hbar}Et} \otimes (x)$$

$$\psi(x, t) = A \exp -\frac{i}{\hbar}Et \exp -\lambda(x - a)^2$$

$$|\psi|^2 = \psi\psi^* = |A|^2 \exp -2\lambda(x - a)^2$$

We computed

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi(x, t)x\psi^*(x, t)dx, \langle p \rangle = \int_{-\infty}^{\infty} \psi \frac{\hbar}{i} \frac{d}{dx} \psi^* = 0$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi x^2 \psi^* dx, \quad \langle p^2 \rangle = \int_{-\infty}^{\infty} \psi \left(\frac{\hbar}{i}\right)^2 \frac{d^2}{dx^2} \psi^* dx$$

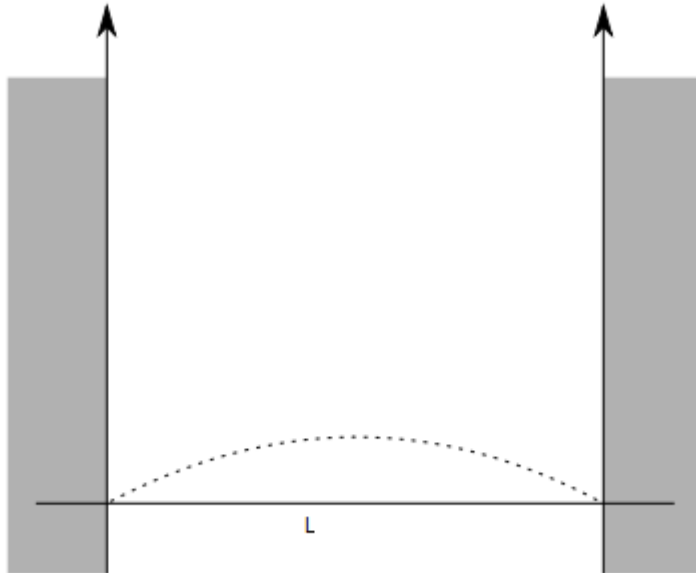
$$\langle x^2 \rangle \sim \frac{1}{\lambda} \quad \langle p^2 \rangle \sim \lambda$$

$$\Delta x \Delta p \sim \hbar$$

$$\frac{\hbar^2}{2m} \Psi'' = E\Psi$$

$$\Psi = A \cos \omega x + B \sin \omega x$$

$$-\omega^2 = \frac{2mE}{\hbar^2}$$



Energy is quantized  
Solving the problem →

$$E_k = \left( \frac{\hbar^2 \pi^2}{2mL^2} \right) k^2$$

$$\psi(x, t) = \sum_{k=1}^{\infty} c_k \sqrt{\frac{2}{L}} \sin\left(\frac{k\pi}{L}x\right) e^{-\frac{i}{\hbar}E_k t}$$

$|c_k|^2$  = probability of finding the system in the state of  $E_k$   
Example

$$\psi(x, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{k\pi}{L}x\right) e^{-\frac{i}{\hbar}E_{10}t} * \frac{1}{4} + \sqrt{\frac{2}{L}} \sin\left(\frac{k\pi}{L}x\right) e^{-\frac{i}{\hbar}E_{28}t} * \sqrt{\frac{15}{16}}$$

$$P(E_{10}) = \left(\frac{1}{4}\right)^2 = \frac{1}{16}$$

$$P(E_{28}) = \frac{15}{16}$$

As soon as one state is measured, wavefunction collapses

$$V = \frac{kx^2}{2} = \frac{m\omega^2}{2}x^2$$

$$\omega = \sqrt{\frac{k}{m}}$$

$$-\frac{\hbar^2}{2m}\psi'' + \frac{m\omega^2}{2}x^2\psi(x) = E\psi(x)$$

→ special function

$$a_{\pm} = \frac{1}{\sqrt{2m}} \left( \frac{\hbar}{i} \frac{d}{dx} \pm im\omega x \right)$$

$$[a_-, a_+] = \hbar\omega, H = \begin{cases} a_+ a_- + \frac{\hbar\omega}{2} \\ a_- a_+ - \frac{\hbar\omega}{2} \end{cases}$$

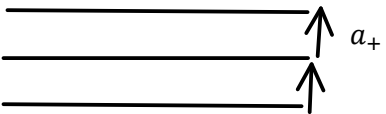
$$[a_{\pm}, H] = \mp \hbar\omega a_{\pm}$$

$$\psi_* \text{ such } H\psi_* = E_*\psi_*$$

$$H(a_{\pm}\psi_*) = (E_* \pm \hbar\omega)(a_{\pm}\psi_*)$$

$$\psi_2 = a_+ a_+ \psi_0 = a_+ \psi_1, E_2 = \frac{5}{2} \hbar \omega$$

$$\psi_1 = a_+ \psi_0, E_1 = \left( \frac{\hbar \omega}{2} + \hbar \omega \right) = \frac{3}{2} \hbar \omega$$

$$\psi_0$$


$$\boxed{a_- \psi_0 = 0} \rightarrow \boxed{\psi_0 = A e^{-\frac{m\omega}{2\hbar} x^2}}$$

$$E_0 = \frac{\hbar \omega}{2}$$

# SS

13 November 2011

12:25

$$-\frac{\hbar^2}{2m} \frac{\delta^2}{\delta x^2} \psi(x, t) + V_x \psi(x, t) = i\hbar \frac{\delta}{\delta x} \psi(x, t)$$

Suppose that

$$\psi(x, t) = e^{-\frac{iE}{\hbar}t} \psi(x)$$

-stationary state

Can be put into schrodinger eq

$$\psi^*(x, t) \times \psi(x, t) = |\psi(x)|^2 \rightarrow \text{probability of the system to be between } (x, x+dx)$$

What we need to impose on a wavefunction?

1. Solves schrodinger eq

$$-\frac{\hbar^2}{2m} \frac{\delta^2}{\delta x^2} \psi(x, t) + V_x \psi(x, t) = i\hbar \frac{\delta}{\delta x} \psi(x, t)$$

2. It has to be differentiable
3. Simple valued
4. Normalizable  $\int_{-\infty}^{\infty} dx |\psi(x)|^2 = 1$

$$\int_{-\infty}^{\infty} e^{-\lambda x^2} dx = \sqrt{\frac{\pi}{\lambda}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\lambda x^2} dx = \sqrt{\frac{\pi}{2\lambda^3}}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) x \psi(x, t) dx$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* x^2 \psi$$

$$(\Delta x) = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

Momentum operator

$$\hat{p} = \frac{\hbar}{i} \frac{\delta}{\delta x}$$

$$\nabla f = \frac{\delta f}{\delta x} \hat{i} + \frac{\delta f}{\delta y} \hat{j}$$

$$\hat{p}\psi(x, t) = \frac{\hbar}{i} \frac{\delta}{\delta x} \psi(x, t)$$

$$\hat{p}^2\psi(x, t) = \hat{p}\hat{p}\psi$$

$$\frac{\hbar}{i} \frac{\delta}{\delta x} \left( \frac{\hbar}{i} \frac{\delta}{\delta x} \psi \right) = -\hbar^2 \frac{\delta^2}{\delta x^2} \psi$$

$$\psi(x, t) = \left( \frac{2\lambda}{\pi} \right)^{\frac{1}{4}} e^{-\frac{i}{\hbar}Et} e^{-\lambda x^2}$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \hbar\sqrt{\lambda}$$

$$\Delta x = \frac{1}{2\sqrt{\lambda}}$$

$$\Delta p = \hbar\sqrt{\lambda}$$

$$\lambda \rightarrow \infty \Delta p \rightarrow \infty$$

$$\lambda \rightarrow 0 \Delta p \rightarrow 0$$

$$\Delta x \Delta p \sim \frac{\hbar}{2}$$

Uncertainty principle

# Angular momentum (spin)

16 November 2011

12:03

Treatment quite similar to the oscillator  $a_+$ ,  $a_-$

Discuss something

$$x' = \gamma(x - vt)$$

$$t' = \gamma\left(t - \frac{vx}{c^2}\right)$$

$$y' = y$$

$$z' = z$$

Lorentz transformations

$$-\frac{\hbar^2}{2m} \frac{\delta^2}{\delta x^2} \psi(x, t) + V(x)\psi(x, t) = i\hbar \frac{\delta}{\delta t} \psi(x, t)$$

Not invariant under Lorentz transformation

Treats time and space differently

$$\frac{\delta^2}{\delta x^2} f(x, y) = \frac{1}{c^2} \frac{\delta^2}{\delta t^2} f(x, t)$$

Is relativistic invariant

Treats time and space the same

$$\psi \sim e^{-\lambda x^2}$$

$$\rightarrow \Delta x \sim \frac{1}{\lambda}$$

$$\Delta p \sim \lambda$$

$$\rightarrow \Delta x \Delta p \sim \hbar$$

Heisenberg uncertainty principle

Suppose that you consider two operators

$$\theta_1, \theta_2$$

These two operators  $\theta_1, \theta_2$  can be measured simultaneously with any precision if and only if  $[\theta_1, \theta_2] = 0$

You cannot measure simultaneously

$$\hat{x}, \hat{p} \rightarrow [\hat{x}, \hat{p}] = i\hbar$$

To measure simultaneously

$$\left. \begin{matrix} \theta_1 \\ \theta_2 \end{matrix} \right\} [\theta_1, \theta_2] = 0$$

$x \rightarrow$  arbitrary precision  $\Delta x \sim 0$

Often some time passes you measure

$$p \Delta p \sim 0$$

This is ok in quantum mechanics

Why is this useful?

In quantum mechanics one describes a system, by giving the values of a set of operators, that commute with each other (complete set of commuting operators)

$$\Delta x \Delta p_x \geq \hbar$$

$$\Delta y \Delta p_y \geq \hbar$$

$$\Delta z \Delta p_z \geq \hbar$$

$$\Delta x \Delta p_y \text{ (not!) } \geq \hbar$$

You can measure  $x$  and  $P_y$  with all the precision you want

$$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$$

$$[x, p_y] = [x, p_z] = [y, p_x] = \dots = [z, p_y] = 0$$

You can measure these with all precision

$$\bar{L} = \bar{R} \times \bar{p}$$

$$\bar{R} = (x\hat{i} + y\hat{j} + z\hat{k})$$

$$\bar{p} = (p_x\hat{i} + p_y\hat{j} + p_z\hat{k})$$

$$\bar{R} \times \bar{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

$$L_x = yp_z - zp_y$$

$$L_y = zp_x - xp_z$$

$$L_z = xp_y - yp_x$$

$$L_x * L_y \neq L_y * L_x$$

### Last time

$\theta_1$  and  $\theta_2$  are two operators  $[x_i, p_x, p_y, p_x^2, \hat{H}, \text{etc}]$   
 You can simultaneously measure  $\theta_1$  and  $\theta_2$  with all precision if

$$[\theta_1, \theta_2] = \theta_1\theta_2 - \theta_2\theta_1 \equiv 0$$

Some commutation relations

$$\left\{ \begin{array}{l} [x, p_x] = [y, p_y] = [z, p_z] = i\hbar \\ [x, y] = [x, z] = [y, z] = 0 \\ [p_x, p_y] = \dots = 0 \\ [x, p_y] = [x, p_z] = \dots = 0 \end{array} \right.$$

$$[AB, C] = A[B, C] + [A, C]B$$

$$AB \cdot C - C \cdot AB = A \cdot (BC - CB) + (AC - CA)B$$

$$ABC - ACB + ACB - CAB = ABC - CAB$$

$$\boxed{[AB, CD] = AC[B, D] + A[B, C] \cdot D + C[A, D]B + [A, C]D \cdot B}$$

Good observables commute with each other such that  $[A, B] = AB - BA = 0$



# Commutation

21 November 2011

14:17

We discuss today are the

$$\begin{aligned} & [L_x, L_z] \\ & [L_x, L_z] \\ & [L_y, L_z] \\ & =? \end{aligned}$$

Will show that they do not commute

$$[L_x, L_y] = [yp_z - xp_y, zp_x - xp_z] = [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z]$$

$$\begin{aligned} [AB, CD] &= AC[B, D] + A[B, C].D + C[A, D]B + [A, C]D.B \\ [yp_z, zp_x] &= yz[p_z, p_x] + y[p_z, z].p_x + z[y, p_x]p_z + [y, z]p_z.p_x \\ yz[p_z, p_x] &= 0 \\ [y, z]p_z.p_x &= 0 \\ z[y, p_x]p_z &= 0 \\ y[p_z, z].p_x &= -i\hbar yp_x \end{aligned}$$

$$[yp_z, zp_x] = -i\hbar$$

$$[zp_y, xp_z] = zx[p_y, p_z] + z[p_y, x]p_z + z[z, p_x]p_y + [z, x]p_xp_z$$

$$[zp_y, xp_z] = i\hbar xp_y$$

$$-[yp_z, xp_z] - [zp_y, zp_x] = 0$$

$$\begin{aligned} [L_x, L_y] &= i\hbar(xp_y - yp_x) \\ &= i\hbar L_z \end{aligned}$$

$$\begin{aligned} [L_x, L_y] &= i\hbar L_z \\ [L_y, L_z] &= i\hbar L_x \\ [L_z, L_x] &= i\hbar L_y \end{aligned}$$

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$[S_x, S_y] = S_x S_y - S_y S_x = \frac{\hbar^2}{4} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \frac{\hbar^2}{4} \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = i\hbar S_z$$

$$[S_y, S_z] = S_y S_z - S_z S_y = \frac{\hbar^2}{4} \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} - \frac{\hbar^2}{4} \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} 0 & 2i \\ 2i & 0 \end{pmatrix} = i\hbar S_x$$

$$[S_z, S_x] = S_z S_x - S_x S_z = \frac{\hbar^2}{4} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} - \frac{\hbar^2}{4} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} = i\hbar S_y$$

Algebra of SU(2)  
Pauli 1929

# Angular momentum

23 November 2011

12:09

$$[AB, C] = A[B, C] + [A, C]B$$

$$L_x = yp_z - zp_y$$

$$L_y = zp_x - xp_z$$

$$L_z = xp_y - yp_x$$

$$\text{Used } [i, p_i] = i\hbar$$

Where  $i=x,y,z$

$$[L_x, L_y] = i\hbar L_z$$

$$[L_y, L_z] = i\hbar L_x$$

$$[L_z, L_x] = i\hbar L_y$$

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$[S_x, S_y] = i\hbar S_z$$

$$[S_y, S_z] = i\hbar S_x$$

$$[S_z, S_x] = i\hbar S_y$$

Notation: sometimes to denote angular momentum, people use J,L,S

S=spin (angular momentum)

L=orbital (angular momentum)

J=total angular momentum

$$\boxed{\vec{J} = \vec{L} + \vec{S}}$$

All satisfy above notation

We said that two operators that do NOT commute and NOT be measured simultaneously with all precision. There is an "uncertainty principle" for any two operators that do NOT commute

$$[\theta_1, \theta_2] \neq 0 \Rightarrow \Delta\theta_1 \Delta\theta_2 \geq \hbar$$

$$[x, p_x] = i\hbar \Rightarrow [\Delta x \Delta p_x \geq \hbar]$$

The "algebra" of angular momentum (commutation relation) tells us that  $L_x, L_y, L_z$  are NOT a good set of observables

$$\text{Let us first introduce } \vec{L}^2 = L_x^2 + L_y^2 + L_z^2$$

$$\vec{L}^2 \equiv L^2$$

Let us study

$$[L^2, L_i]$$

$i=x,y,z$

$$[L^2, L_z] = [L_x^2 + L_y^2 + L_z^2, L_z] = [L_x^2, L_z] + [L_y^2, L_z] + [L_z^2, L_z]$$

$$[L_x^2, L_z] = L_x[L_x, L_z] + [L_x, L_z]L_x = L_x i\hbar L_y + i\hbar L_y L_x = -i\hbar(L_y L_x + L_x L_y)$$

$$[L_y^2, L_z] = i\hbar(L_x L_y + L_y L_x)$$

$$[L_z^2, L_z] = L_z[L_z, L_z] + [L_z, L_z]L_z = 0$$

$$[L^2, L_z] = -i\hbar(L_y L_x + L_x L_y) + i\hbar(L_x L_y + L_y L_x) + 0 = 0$$

$$[L^2, L_i] = 0$$

This tells us that two good observables two good operators measure one

$$\begin{pmatrix} L^2 \text{ and } L_z \\ L^2 \text{ and } L_y \\ L^2 \text{ and } L_x \end{pmatrix}$$

In all the books, people choose

### $L^2$ and $L_z$

Exactly as we did in the oscillator, we will define two new operators

$$L_+ = L_x + iL_y$$

$$L_- = L_x - iL_y$$

$$[L_z, L_+] = [L_z, L_x + iL_y] = [L_z, L_x] + i[L_z, L_y] = \hbar(L_x + iL_y) = \hbar L_+$$

$$[L_z, L_-] =$$

$$[L^2, L_+] = [L^2, L_x + iL_y] = [L^2, L_x] + [L^2, L_y] = 0$$

$$[L^2, L_-] = 0$$

$$[J_x, J_y] = i\hbar J_z$$

etc

$$[L_y, L_z] = i\hbar L_x$$

$$[L_z, L_x] = i\hbar L_y$$

Convention: Use  $J_z$  and  $J^2$  as observables

$$J_{\pm} = J_x \pm iJ_y$$

$$J^2 = J_x^2 + J_y^2 + J_z^2$$

And

$J_z$

$$J_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$J_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$J_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$\psi_{l,m}$

$l \rightarrow J^2, m \rightarrow J_z$

$$J^2 \psi_{l,m} = \hbar^2 l(l+1) \psi_{l,m}$$

$$J_z \psi_{l,m} = \hbar m \psi_{l,m}$$

$m: -l, \dots, l$

Limits of (1)

Quantum numbers  $l$  and  $m$

Consider a particle of spin  $1/2 \equiv$  electron, proton, neutron, quark

$$\psi_{l,m}; \quad l = \frac{1}{2}$$

$$m = -\frac{1}{2}, \frac{1}{2}$$

Two states

$$\psi_{\frac{1}{2}, \frac{1}{2}}$$

And

$$\psi_{\frac{1}{2}, -\frac{1}{2}}$$

Spin 1  $\rightarrow$  photons

$$\psi_{1,1}$$

$$\psi_{1,0}$$

$$\psi_{1,-1}$$

Spin 2  $\rightarrow$  gravitons

$$\psi_{2,2}$$

$\psi_{2,1}$   
 $\psi_{2,0}$   
 $\psi_{2,-1}$   
 $\psi_{2,-2}$

$J_{\pm}$  = ladder operators  
 Change between states for m

$$J_+ = J_x + iJ_y = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$J_- = J_x - iJ_y = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$J^2 = J_x^2 + J_y^2 + J_z^2 = \left[ \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right]^2 + \left[ \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right]^2 + \left[ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right]^2 = \dots = \frac{3}{4} \hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$J_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$J_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$J_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; v_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$J_z v_1 = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$J_z v_2 = \frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$J^2 v_1 = \frac{3}{4} \hbar^2 v_1$$

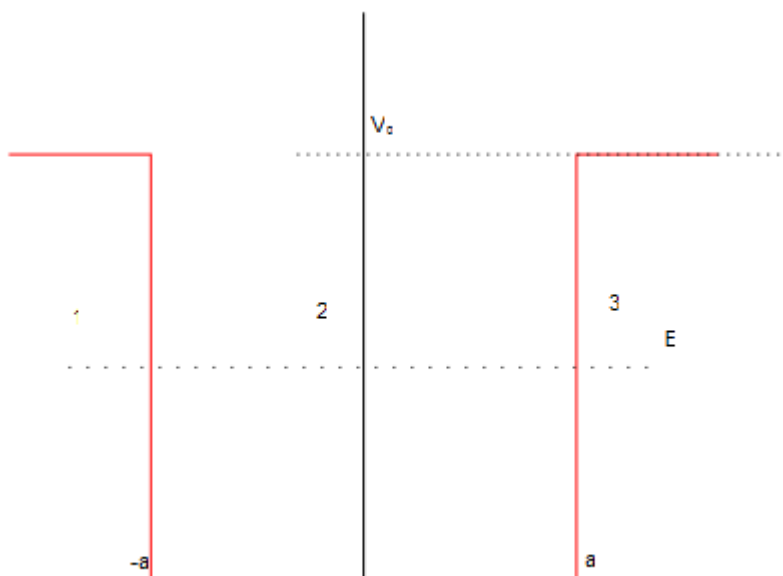
$$J^2 v_2 = \frac{3}{4} \hbar^2 v_2$$

$$J_+ v_1 = \hbar \cdot 0$$

$$J_+ v_2 = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar v_1$$

$$J_- v_1 = \hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$J_- v_2 = 0$$



Schrodinger eq in region 1 (left) and 3 (right)

$$-\frac{\hbar^2}{2m}\psi''(x) + V_0\psi(x) = E\psi_0$$

$$\rightarrow \boxed{\psi'' + \frac{2m}{\hbar^2}(E - V_0)\psi(x) = 0}$$

In 2

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

$$\rightarrow \boxed{\psi'' + \frac{2m}{\hbar^2}\psi(x) = 0}$$

$$\psi'' + \omega^2\psi = 0 \rightarrow A \cos \omega x + B \sin \omega x$$

$$\psi'' - \omega^2\psi = 0 \rightarrow A e^{+\omega x} + B e^{-\omega x}$$

In regions 1 and 3

$$\psi'' + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$

$$\psi'' - \omega^2\psi$$

$$\boxed{\omega^2 = \frac{2m}{\hbar^2}(V_0 - E)}$$

In 1

$$\psi_1 = A e^{\omega_1 x} + B e^{-\omega_1 x}$$

In 3

$$\psi_3 = C e^{\omega_1 x} + D e^{-\omega_1 x}$$

In 2

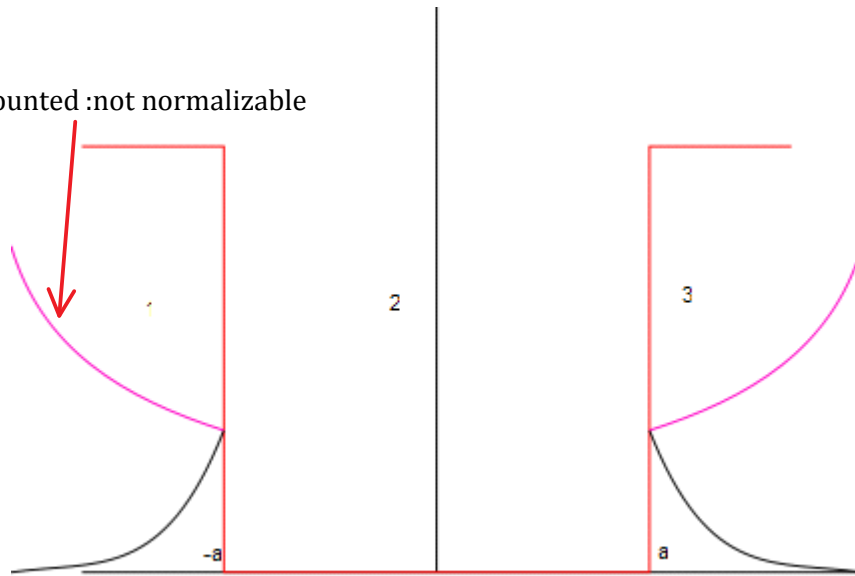
$$\psi'' + \omega_2^2\psi = 0$$

$$\omega_2^2 = \frac{2m}{\hbar^2}E$$

$$\boxed{\psi_2 = Q \cos \omega_2 x + F \sin \omega_2 x}$$

Discounted - not normalizable

Discounted :not normalizable



Schrodinger eq in 1, in 3

In region 1

$$\psi_1 = Ae^{\omega_1 x}$$

In region 2

$$\psi_2 = Q \cos \omega_2 x + F \sin \omega_2 x$$

In region 3

$$\psi_3 = De^{-\omega_1 x}$$

$$\omega_1^2 = \frac{2m}{\hbar^2} (V_0 - E)$$

$$\omega_2^2 = \frac{2m}{\hbar^2} E$$

A wave function needs to be continuous and differentiable

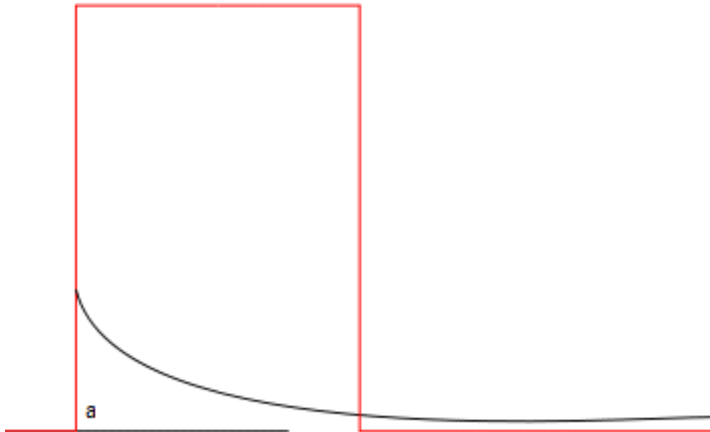
- i.  $\psi_1(x = -a) = \psi_2(x = -a)$
  - ii.  $\psi_1'(x = -a) = \psi_2'(x = -a)$
  - iii.  $\psi_2(x = a) = \psi_3(x = a)$
  - iv.  $\psi_2'(x = a) = \psi_3'(x = a)$
- i)  $Ae^{-\omega_1 a} = Q \cos \omega_2 a - F$
  - ii)  $A\omega_1 e^{-\omega_1 a} = Q \sin \omega_2 a + F \cos \omega_2 a$
  - iii)  $\omega_2 (Q \cos \omega_2 a + F \sin \omega_2 a) = D\omega_1 e^{-\omega_1 a}$
  - iv)  $\omega_2 (Q \cos \omega_2 a + F \sin \omega_2 a) = -D\omega_1 e^{\omega_1 a}$

A,Q,F,D

Unknowns

4 equations: put in mathematica

$$\int_{-\infty}^{-a} \psi \psi^* + \int_{-a}^a \psi \psi^* + \int_a^{\infty} \psi \psi^* = 1$$



### Quantum tunnelling

Lagrangian → definition

$$L = T - V$$

where

$$T = \frac{m\dot{x}^2}{2}$$

V=potential

1. Free Particle →  $V = 0$  →  $L = \frac{m\dot{x}^2}{2}$

2. Oscillator

$$\rightarrow V = \frac{Kx^2}{2} \rightarrow L = \frac{m\dot{x}^2}{2} - \frac{kx^2}{2}$$

$$F = -kx$$

Action,

$$S = \int_{t_0}^t L dt$$

Momentum action principle

impose → minimize the action  $\delta S = 0$

→ find some eqs Euler Lagrange eps

$$\frac{d}{dt} \left( \frac{\delta L}{\delta \dot{x}} \right) = \frac{\delta L}{\delta x}$$

$$\frac{\delta L}{\delta \dot{x}} \rightarrow \text{Free } m\dot{x} \rightarrow \frac{d}{dt}(m\dot{x}) = m\ddot{x} + \dot{m}\dot{x}$$

$$\frac{\delta L}{\delta x} \rightarrow \text{Free } 0$$

$$\text{Free particle } m\ddot{x} = 0$$

$$\text{Oscillator } m\ddot{x} = -kx$$

Much more complicated if mass ≠ constant

### Interference + diffraction

$$\psi = \psi_1 + \psi_2$$

$$P = |\psi_1|^2 + |\psi_2|^2 + 2\psi_1\psi_2$$

$$\psi_1\psi_2^* + \psi_2\psi_1^*$$

$$P = P_1 + P_2 + \text{Interference term}$$

$$L = T - V = \frac{m\dot{x}^2}{2} - V(x)$$

$$\boxed{\frac{d}{dt} \left( \frac{\delta L}{\delta \dot{x}} \right) = \frac{\delta L}{\delta x}}$$

Action

$$S = \int_{t_0}^{t_t} L dt$$

2 slit

$$\psi_A = \psi_1 + \psi_2$$

$$I = |\psi_A|^2 = |\psi_1 + \psi_2|^2 = \psi_1^2 + \psi_2^2 + 2\psi_1\psi_2$$

$$2\psi_1\psi_2 = \text{interference}$$

3 slit

$$\psi_A = \psi_1 + \psi_2 + \psi_3$$

$$I = |\psi_1 + \psi_2 + \psi_3|^2$$

4 slit

$$\psi_A = \psi_1 + \psi_2 + \psi_3 + \psi_4$$

$$I = |\psi_1 + \psi_2 + \psi_3 + \psi_4|^2$$

Electrons

$$\psi_A = \psi_1 + \psi_2$$

Wavefunction at x=A

$$\text{Prob (electron at A)} = |\psi_A|^2$$

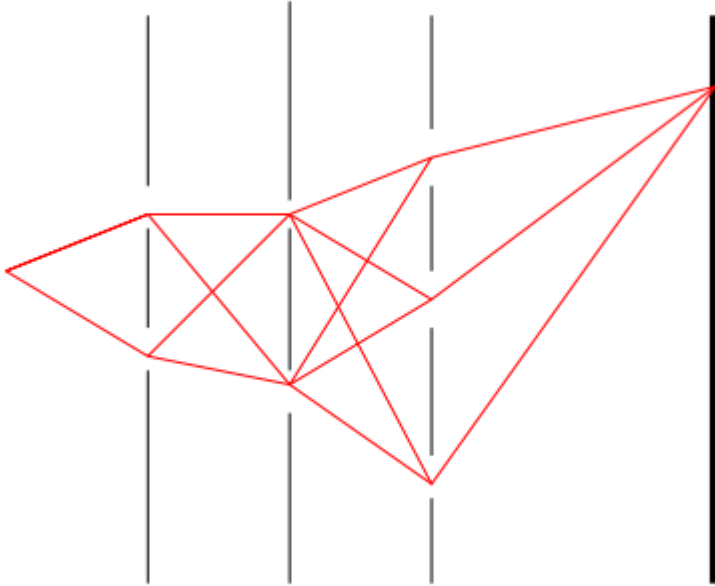
$$= |\psi_1 + \psi_2|^2 = |\psi_1|^2 + |\psi_2|^2 + \psi_1\psi_2^* + \psi_2\psi_1^*$$

$$\psi_A = \sum \psi_i(x_i)$$

$$\boxed{P(A) = |\sum \psi_i|^2}$$

$\psi_A$  = sum over all paths to get to the point A





$$\psi_A = \sum \psi_{ijk}$$

$\psi(x_1 t_1, x_2 t_2) = \sum_{\psi_i}$  all possible paths/ways that go from  $(x_1 t_1) \rightarrow (x_2 t_2)$

$$\text{Amplitude}(x_1, t_1, x_2, t_2) = \int DX \exp -\frac{i}{\hbar} \int_{t_1}^{t_2} L dt$$

DX means sum over ALL paths

Equivalent to schrodinger eq for  $L = \frac{m\dot{x}^2}{2} - V(x)$

1. Classical limit  $\hbar \rightarrow 0$

$$\Delta x \Delta p \geq \hbar$$

$$\exp -\frac{i}{\hbar} \int_{t_1}^{t_2} L dt \rightarrow \sin + \cos$$

$$A \cong \exp -\frac{i}{\hbar} S_{\text{classical}}$$

$S \rightarrow \text{path}$

All this course we worked with NON relativistic quantum mechanics

# Exam

Mon Jan 16 2pm

Email carlos if you want to redo any of the mid terms

Schrodinger eq will be written in exam- don't need to memorize

Given a  $\psi(x, t) \rightarrow$

$$\begin{aligned} &\langle x \rangle \\ &\langle x^2 \rangle \\ &\langle p \rangle \\ &\langle p^2 \rangle \end{aligned}$$

$$\Delta x \Delta p \geq \hbar$$

Operators

$$|\theta_1, \theta_2, \dots, \theta_n\rangle$$

Good operators if

$$[\theta_1, \theta_2] \Rightarrow \text{all precision etc}$$

Good observables

$$(L_x, L_z)$$

$$(p_x, p_y)$$

Angular momentum

$L_i$  etc

$$L_x = yp_z - zp_y \text{ etc}$$

$$L^2 = L_i^2$$

Where  $i=x,y,z$

$$[L_x, L_y] = i\hbar L_z$$

etc

$$L_{\pm} = \text{effects on the states}$$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}; \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$J_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$

$$J_- \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$J_+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$J_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

$$J_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; J_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

$$J_z = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

$$(J_z, J^2)$$

Oscillator

$$-\frac{\hbar}{2m} \frac{\delta^2}{\delta x^2} \psi + V\psi = i\hbar \frac{\delta}{\delta t} \psi$$

$$V = \frac{kx^2}{2}$$

$$a_+ = \frac{1}{\sqrt{2m}} \left( \frac{\hbar}{i} \frac{d}{dx} + im\omega x \right)$$

$$a_- = \frac{1}{\sqrt{2m}} \left( \frac{\hbar}{i} \frac{d}{dx} - im\omega x \right)$$

$$[a_+, a] = ?$$

$$[a_{\pm}, H] = ?$$

Spectrum discrete

$$E_m = \left( n + \frac{1}{2} \right) \hbar \omega$$

$$\psi \Rightarrow \boxed{a_- \psi_0 = 0} \rightarrow \text{solved}$$

$$\psi_0 = e^{-x^2}$$

$$\psi_1 = a_+ \psi_0$$

$$\psi_2 = a_+ a_+ \psi_0$$

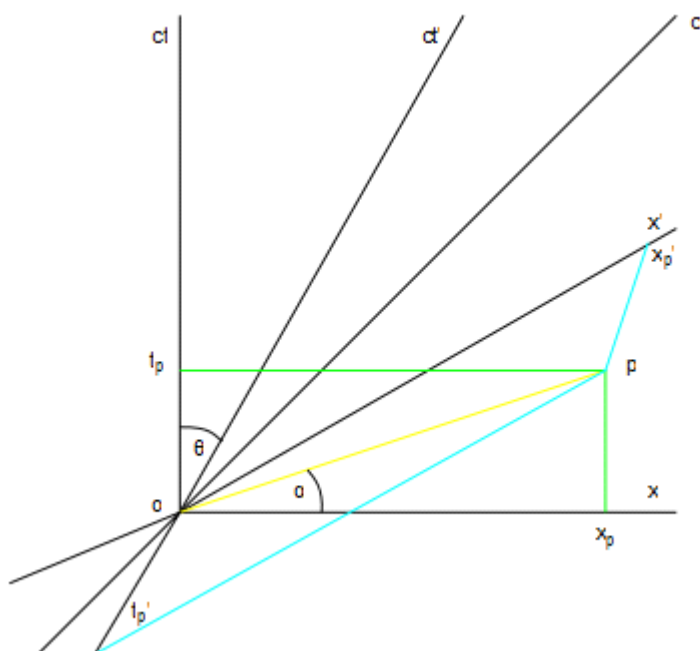
Etc

Go over these things to ensure understanding

# FTL

27 November 2011

15:12



Op is a faster than light path

In frame S, op is forwards in time  $t_p > t_0$

In frame S', 0P is backwards in time,  $t'_p < t'_0$

⇒ If a faster than light signal is possible, Then in some frames it is forwards in time, but in other frames it is backwards in time

$$\tan \theta = \frac{v}{c}$$

$$\tan \alpha = \frac{c}{u}$$

Where u is the speed of the tachyon

Backwards in time in S' if the relativity velocity of the frames satisfies

$$\tan \theta > \tan \alpha$$

$$\Rightarrow \frac{v}{c} > \frac{c}{u} \Rightarrow v > \frac{c^2}{u}$$

Directly from Lorentz transformation

For 0p,

$$ct' = \gamma \left( ct - \frac{v}{c} x \right)$$

$$x' = \gamma \left( x - \frac{v}{c} ct \right)$$

Speed of tachyon  $u = \frac{x}{t}$

$$t' < 0 \text{ if } ct - \frac{v}{c} x < 0$$

$$\Rightarrow ct \left( 1 - \frac{v}{c^2} \frac{x}{t} \right) < 0$$

$$\left( 1 - \frac{v}{c^2} \frac{x}{t} \right) \Rightarrow 1 - \frac{v}{c^2} u$$

$$\Rightarrow v > \frac{c^2}{u}$$

So far, this is not a terminal problem

The problem is that once we accept faster than light/backwards in time in some frame is possible, Postulate I says that it is possible in all inertial frames in particular, it implies that if 0p is possible, then so is motion PQ



Closed path  $OPQ$  is incompatible with causality (Grandfather paradox)

# Problem Sheets

21 November 2011

15:18

## Sheet 3

1. Track =  $1.05 * 10^{-9}m$

Speed =  $0.992 * 3 * 10^8 ms^{-1}$

⇒ lifetime in LAB FRAME

$$= \frac{1.05 * 10^{-9}}{0.992 * 3 * 10^8} = 3.53 * 10^{-18}sec$$

Lifetime in REST FRAME

$$= \frac{1}{\gamma} (3.53 * 10^{-18}) = 0.445 * 10^{-18}sec$$

$$S^2 = -c^2t^2 + x^2 \text{ lab}$$

$$= -c^2t'^2 \text{ rest}$$

$$\Rightarrow t'^2 = t^2 - \frac{x^2}{c^2}$$

$$\Rightarrow t' = t \sqrt{1 - \frac{v^2}{c^2}}$$

$$= \gamma^{-1}t$$

2. Lifetime in rest frame =  $26 * 10^{-9}s$

At 0.99c

$$\gamma = \frac{1}{\sqrt{1 - 0.99^2}} = 7.1$$

$$\Rightarrow \text{lifetime in lab/earth frame} = \gamma(26 * 10^{-9}) = 184 * 10^{-9}s$$

$$\text{Distance} = 1.84 * 10^{-7} * 0.99 * 3 * 10^8m = 54.6m$$

$$1 - \frac{v^2}{c^2} = \left(1 + \frac{v}{c}\right) \left(1 - \frac{v}{c}\right)$$

$$1 - 0.99^2 = (1.99)(0.01) = 0.02$$

$$\gamma = \frac{1}{\sqrt{0.02}} = \frac{1}{\sqrt{0.02}} = \frac{10}{\sqrt{2}} \approx \frac{10}{1.4} = 7$$

3.

i. Earth time when astronaut reaches VEGA

$$= \frac{26}{0.99} yrs = 26 * 26 yrs$$

$$\frac{1}{0.99} = \frac{1}{1 - 0.01} = (1 - 0.01)^{-1}$$

$$= 1 + 0.01 + 0(0.01)^2 = 1.01$$

ii. Time to receive radio signal =  $26.26 + 26 = 52.26 yrs$

iii. Astronaut time at VEGA =  $\frac{1}{\gamma} 26.26 = 3.7 yrs$

$$\gamma = \frac{1}{\sqrt{1 - 0.99^2}} = 7.1$$

$$s^2 = -c^2t'^2$$

$$= -c^2t^2 + x^2$$

$$t'^2 = t^2 - \frac{x^2}{c^2} = t^2 \left(1 - \frac{v^2}{c^2}\right)$$

$$t'^2 = (26.26)^2 - 26^2$$

$$= (26 + 0.26)^2 - 26^2 \cong (52 * 0.26) = 13$$

4.

i. Length earth =  $\frac{1}{\gamma}$  plane length =  $(1 - 2.2 * 10^{-12})L_{plane}$

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$= \left(1 - \frac{v^2}{c^2}\right)^{\frac{1}{2}}$$

$$\cong 1 + \frac{1}{2} \frac{v^2}{c^2} + \dots$$

$$v = 630 \text{ m/s}$$

$$c = 3 \cdot 10^8 \text{ m/s}$$

$$\frac{v}{c} = \frac{630}{3 \cdot 10^8} = 2.1 \cdot 10^{-6}$$

$$= 1 + 2.2 \cdot 10^{-12}$$

Change in plane length as measured on earth/length

$$= 2.2 \cdot 10^{-12} L/L$$

$$= 2.2 \cdot 10^{-12}$$

Sheet 2

1) 1st half

Invariant spacetime interval

$$S^2 = -c^2 t^2 + x^2$$

Earth frame

$$S^2 = -5^2 + 4.9^2$$

Astronaut frame

$$s^2 = -c^2 \tau^2$$

$$\Rightarrow \tau^2 = 5^2 - 4.9^2$$

$$= 9.9 \cdot 0.1$$

$$= 0.99$$

$$\tau = \sqrt{0.99}$$

$$= 0.995$$

Total =  $0.995 \cdot 2 = 1.99 \text{ yrs}$

OR

$$\frac{v}{c} = \frac{4.9}{5} = 0.98$$

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{1}{0.199}$$

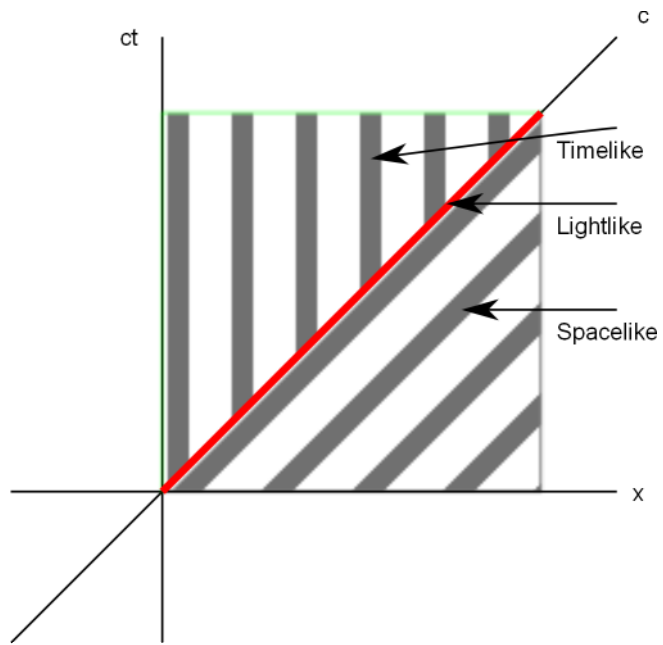
Total time in astronaut frame

$$= \gamma^{-1} \cdot \text{earth time}$$

$$= 0.199 \cdot 10 = 1.99 \text{ yrs}$$

2) Simultaneity- straight out of lecture notes

3) Timelike, lightlike, spacelike



As long as motion is timelike, motion is always forwards in time



# 1 Vectors & Newtonian dynamics

04 October 2011

10:11

Position vector

$$\vec{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

Any vector

$$\vec{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

Index notation

Scalar product of vectors

$$\vec{u} \cdot \vec{v} = u_1 v_1 + u_2 v_2 + u_3 v_3 = \sum_{i=1}^3 u_i v_i$$

Now introduce Kronecker delta symbol

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

Consider this as a matrix

$$\delta_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \delta_{11} & \delta_{12} & \delta_{13} \\ \delta_{21} & \delta_{22} & \delta_{23} \\ \delta_{31} & \delta_{32} & \delta_{33} \end{pmatrix}$$

Scalar product is

$$\vec{u} \cdot \vec{v} = \sum_{i=1}^3 \sum_{j=1}^3 \delta_{ij} u_i v_j$$

Matrix form

$$\vec{u} \cdot \vec{v} = (u_1 \quad u_2 \quad u_3) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

"Einstein sum convention

So just write  $u_i v_i$  instead of  $\sum_{i=1}^3 u_i v_i$

Notice that this is what we did with the metric (distance relation)

$$ds^2 = dx^2 + dy^2 + dz^2 = \delta_{ij} dx_i dx_j$$

^scalar product                                      ^metric

In general,  $ds^2 = g_{ij} dx_i dx_j$

Where the metric  $g_{ij}$  determines the shape of the space eg 3-sphere, hyperboloid

Flat Euclidean space  $g_{ij} = \delta_{ij}$

Rotations

Restrict to 2 dimensions for simplicity

Vector

$$\vec{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = v_1$$

Under rotation

$$\vec{v} \rightarrow \vec{v}' = \begin{pmatrix} v'_1 \\ v'_2 \end{pmatrix} = v'_1$$

$$v'_i = R_{ij} v_j = \sum_{j=1}^2 R_{ij} v_j$$

In matrix notation

$$\begin{pmatrix} v'_1 \\ v'_2 \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$$

$$R_{ij} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

R has a special property

$$R^T R = 1$$

$$\begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

We say that R is "orthogonal"

In 3 dims,  $R_{ij}$  where  $i, j = 1, 2, 3$  (3x3 matrix)

Still Orthogonal  $R^T R = 1$

N dimensions  $\rightarrow \frac{1}{2}N(N-1)$  angles

"Group theory"- mathematics of symmetry

Frame of reference

This is a system of measuring space and time, set up by observers with identical motions

In general, the description of events will be different in different frames, BUT underlying reality is the same

Eg

One frame S which is fixed relative to the earth

Another frame S' could be aboard a plane

Each frame will assign position to an event  $S \rightarrow (x, y, z)$  and time  $t$   $S' \rightarrow (x', y', z')$  **and time t**

### Newtonian dynamics

Essential feature is the special role given to inertial frames of reference i.e. fixed, or moving with uniform velocity NOT accelerating.

Postulates

1. The laws of dynamics are the same in all inertial frames (all inertial frames are equivalent)

This is a relativity principle- it means there is no absolute rest frame, only relative motion is important

2. Since all inertial frames are equivalent, the simplest effect of an interaction (force) is to produce an acceleration

$$\rightarrow \vec{F} = m \frac{d^2 \vec{x}}{dt^2}$$

Forces change acceleration, not velocity

3. Dynamics takes place in flat Euclidean space  $\Rightarrow$  laws of dynamics are invariant under rotations & translations deep theorem (Noether's theorem)

Translation invariance  $\rightarrow$  momentum is conserved

Rotation invariance  $\rightarrow$  angular momentum conserved

### Galilean transformations

Relate measurements in different inertial frames

(look at 1 space dim for simplicity)

"moving" frame (s' with velocity v) has coords (x', t')

Stationary frame (s) has coords (x, t)

In S, event p has coordinates  $(x_p, t_p)$

Clearly,  $x'_p = x_p - vt_p$

Assume  $t'_p = t_p$

Applies to any event P, so we have the general relation between coordinates in frames S and S' (galilean transformations)

$$\begin{cases} t' = t \\ x' = x - vt \end{cases}$$

$$\text{in 3 dim } \begin{cases} t' = t \\ \vec{x}' = \vec{x} - \vec{v}t \end{cases}$$

Invariance of equation of motion

$$\vec{F} = m \frac{d^2 \vec{x}}{dt^2} \text{ should have } \vec{F} = m \frac{d^2 \vec{x}'}{dt'^2}$$

$$\Rightarrow \vec{F} = m \frac{d^2 \vec{x}'}{dt'^2} = m \frac{d^2}{dt^2} (\vec{x} - \vec{v}t) = m \frac{d^2 \vec{x}}{dt^2}$$

Postulate 1 holds

## 2 Space and time in special relativity

10 October 2011  
10:45

Newtonian picture is changed radically in special relativity (Einstein 1905)

Special relativity is based on the following postulates

Postulate 1A

The laws of physics are the same in all inertial frames

Postulate 1B

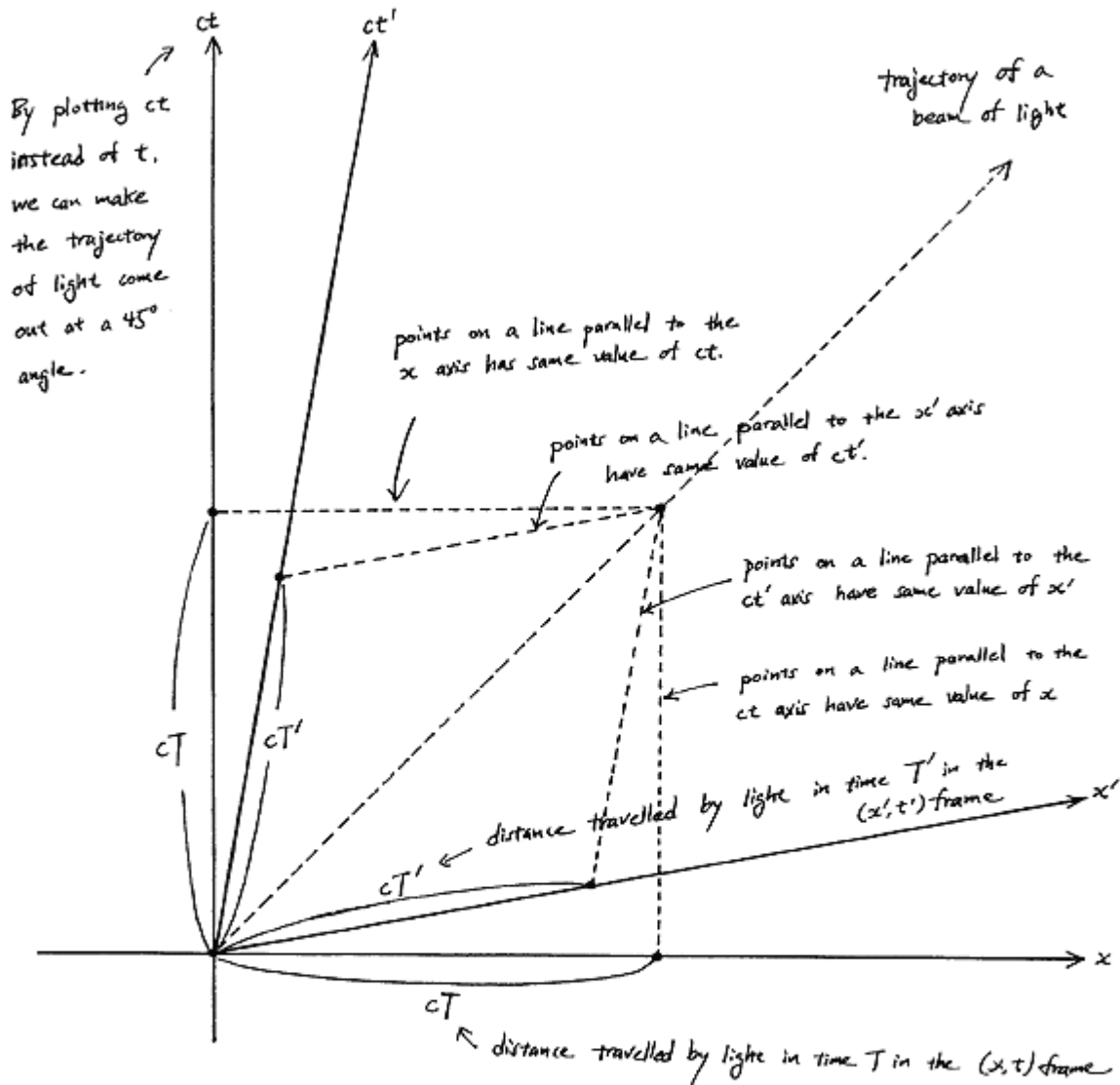
The speed of light is the same in all inertial frames

Note Postulate 1B introduces a new fundamental constant  $c$  into physics. (compare with quantum mechanics, scale  $h$ )

Postulate 1A extends relativity principle (equivalence of inertial frames) to all of physics in particular including electromagnetism, not just particle dynamics

To satisfy postulate 1B, we need to change our ideas of space and time

Use  $ct$  and  $x$  as axes- both have dimensions of length



★ The Galilei Transformation tilts the  $t'$  axis.

★ The Lorentz Transformation tilts both  $x'$  and  $t'$  axes.

Measure speed of light in new frame S'. To keep speed of light = c, need to change both axes (ct', x') both different from (ct, x)

⇒ time is different in different inertial frames

### Lorentz Transformations

These show how space and time coordinates are related in frames S and S' with relative velocity v

[For simplicity, assume  $\vec{v}$  is along x-axis]

Postulate 1B

$$x' = \gamma \left( x - \frac{v}{c} ct \right)$$

$$ct' = \gamma \left( ct - \frac{v}{c} x \right)$$

\*

Check the speed of light

$$\text{Vel in } S = \frac{x}{t} = u$$

$$\text{Vel in } S' = \frac{x'}{t'} = \frac{\gamma \left( x - \frac{v}{c} ct \right)}{\gamma \left( t - \frac{v}{c^2} x \right)} = u'$$

$$\frac{\gamma \left( \frac{x}{t} - v \right)}{\gamma \left( 1 - \frac{v}{c^2} \frac{x}{t} \right)}$$

$$\Rightarrow \boxed{u' = \frac{u - v}{1 - \frac{uv}{c^2}}}$$

This formula relates a velocity u measured in S to the velocity u' measured in S'

Note  $u' \approx u - v$  only when  $u, v \ll c$

Postulate 1B says that if  $u=c$ , then  $u'=c$

Set  $u=c$

$$\Rightarrow u' = \frac{c - v}{1 - \frac{cv}{c^2}} = c$$

So Postulate 1B is satisfied by transformations

NB this would be true for any choice of gamma

Postulate 1A

This means we must have the same transformation from S' to S

$$x = \gamma \left( x' + \frac{v}{c} ct' \right)$$

$$ct = \gamma \left( ct' + \frac{v}{c} x' \right)$$

\*\*

NB change sign of relative velocity

Check consistency of \* and \*\*

$$x = \gamma^2 \left( x - vt + v \left( t - \frac{v}{c^2} x \right) \right) = \gamma^2 \left( 1 - \frac{v^2}{c^2} \right) x$$

$$ct = \gamma^2 \left( ct - \frac{v}{c} x + \frac{v}{c} (x - vt) \right) = \gamma^2 \left( 1 - \frac{v^2}{c^2} \right) ct$$

$$\Rightarrow \gamma^2 = \frac{1}{1 - \frac{v^2}{c^2}}$$

$$\Rightarrow \gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

So Postulate 1A shows that the scale factor  $\gamma$  is not arbitrary (as allowed by Postulate 1B alone) but is velocity dependent,

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

To summarise

The Lorentz transformations are

$$x' = \gamma \left( x - \frac{v}{c} ct \right)$$

$$t' = \gamma \left( t - \frac{v}{c^2} x \right)$$

Where

$$\gamma(v) = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

NB- transverse space coordinates are unchanged

Note that these reduce to Galilean transformations when  $c \rightarrow \infty$

### Minkowski Spacetime

Since Lorentz transformations mix space and time, the geometry relevant for special relativity is 4-dimensional spacetime

However, 4-dim Minkowski spacetime is NOT just Euclidean space

Recall the Lorentz transformations

$$ct' = \gamma \left( ct - \frac{v}{c} x \right)$$

$$x' = \gamma \left( x - \frac{v}{c} ct \right)$$

So both  $x$  and  $t$  are changed under a change of frame  $S$  to  $S'$

But something is left invariant.

Invariant is

$$S^2 = -c^2 t^2 + x^2$$

$$(\text{in 3d } S^2 = -c^2 t^2 + x^2 + y^2 + z^2)$$

Check

$$S'^2 = -c^2 t'^2 + x'^2$$

$$= -\gamma^2 \left( ct - \frac{v}{c} x \right)^2 + \gamma^2 \left( x - \frac{v}{c} ct \right)^2$$

$$= \gamma^2 \left[ -c^2 t^2 + 2vxt - \frac{v^2}{c^2} x^2 + x^2 - 2vxt + \frac{v^2}{c^2} c^2 t^2 \right]$$

$$= -\gamma^2 \left( 1 - \frac{v^2}{c^2} \right) c^2 t^2 + \gamma^2 \left( 1 - \frac{v^2}{c^2} \right) x^2$$

$$= -c^2 t^2 + x^2$$

$$\text{Since } \gamma^2 = \frac{1}{1 - \frac{v^2}{c^2}}$$

So the combination  $S^2 = -c^2 t^2 + x^2 + y^2 + z^2$  is always the same, no matter which frame of reference we use

Analogue of distance in 3d Euclidean space

Call  $s^2$  the (square of the) spacetime interval between origin and point

Introduce position 4-vector  $x = \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}$

Generalising 3-vector  $x^i = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, i = 1, 2, 3$

$$x^\mu = \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}, \mu = 0, 1, 2, 3$$

0=time; 1,2,3=space

A Lorentz transformation is  $x^\mu \rightarrow x'^\mu$

Where

$$x'^\mu = L^\mu_\nu x^\nu \quad \text{where } L^\mu_\nu = \begin{pmatrix} \gamma & -\frac{v}{c}\gamma & 0 & 0 \\ -\frac{v}{c}\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Generalizes rotations in 3d space

$$x'^i = R_j^i x^j$$

$3 * 1 \quad 3 * 3 \quad 3 * 1$

We can write the spacetime interval as

$$S^2 = (ct \ x \ y \ z) \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}$$

$$= x^\mu g_{\mu\nu} x^\nu = x^T g x \text{ in matrix notation}$$

$$\text{Where } g_{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

This generalizes 3d distance  $S^2 = x^T 1 x = x^i \delta_{ij} x^j$

The 4x4 matrix  $g_{\mu\nu}$  specifies the spacetime interval in Minkowski spacetime it is called the metric

Now re-check that  $S^2$  is invariant under Lorentz transformations

$$S^2 = g_{\mu\nu} x^\mu x^\nu$$

Lorentz tranf  $x^\mu \rightarrow x'^\mu = L^\mu_\nu x^\nu$

Check

$$S^2 = g_{\mu\nu} x'^\mu x'^\nu$$

$$= g_{\mu\nu} L^\mu_\rho x^\rho L^\nu_\sigma x^\sigma$$

$$g_{\mu\nu} x^\mu x^\nu = g_{\rho\sigma} x^\rho x^\sigma$$

$\Rightarrow S^2$  is invariant if

$$g_{\mu\nu} L^\mu_\rho L^\nu_\sigma = g_{\rho\sigma}$$

Matrix notation

$$S^2 = x'^T g x'$$

$$= x^T L^T g L x$$

$$= x^T g x \text{ if } S^2 \text{ is invariant}$$

$$\Rightarrow \boxed{L^T g L = g}$$

CHECK

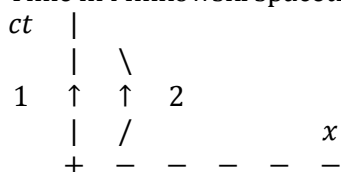
$L^T g L$

$$= \begin{pmatrix} \gamma & -\frac{v}{c}\gamma & 0 & 0 \\ -\frac{v}{c}\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \gamma & -\frac{v}{c}\gamma & 0 & 0 \\ -\frac{v}{c}\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \gamma & -\frac{v}{c}\gamma & 0 & 0 \\ -\frac{v}{c}\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} -\gamma^2 \left(1 - \frac{v^2}{c^2}\right) & 0 & 0 & 0 \\ 0 & \gamma^2 \left(1 - \frac{v^2}{c^2}\right) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = g$$

Time in Minkowski spacetime compare 2 paths through Minkowski spacetime



What does an observer measure as "time"

"proper time" as measured in a frame of reference where the observer is at rest is  $t$  where

$$s^2 = -c^2 t^2$$

Infinitesimally,

$$ds^2 = -c^2 dt^2$$

So observer 1 measures time elapsed as  $t$  where  $\int_{path 1} ds$  is the spacetime interval and

$$ds^2 = -c^2 dt^2$$

Similarly for observer 2, there the spacetime interval is  $\int_{path 2} ds$

But spacetime interval along path 2 is less than path 1

Because  $ds^2 = -c^2 dt^2 + dx^2 \Rightarrow$  path with biggest value of  $S$  is the one where there is no motion in the space direction

This is the famous "astronaut paradox" astronaut 1 stays of earth

Astronaut 2 goes on a fast round trip to alpha centauri and back. When they meet back on earth astronaut 2 is younger then astronaut 1

This is not a paradox because paths 1 and 2 are genuinely different. Path 1 is inertial, path 2 is not. So there is no symmetry between them-> cannot say path 2 is at rest and path 1 moves



# 3 Measurement of space and time

18 October 2011  
10:45

## 3.1 Simultaneity

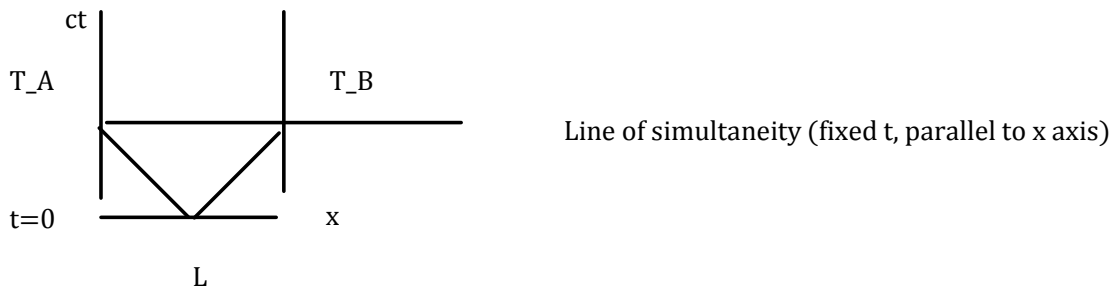
Simultaneity is not an absolute property of two events but depends on the frame of reference  
Operational definition of simultaneity

Consider a rod of length  $L$

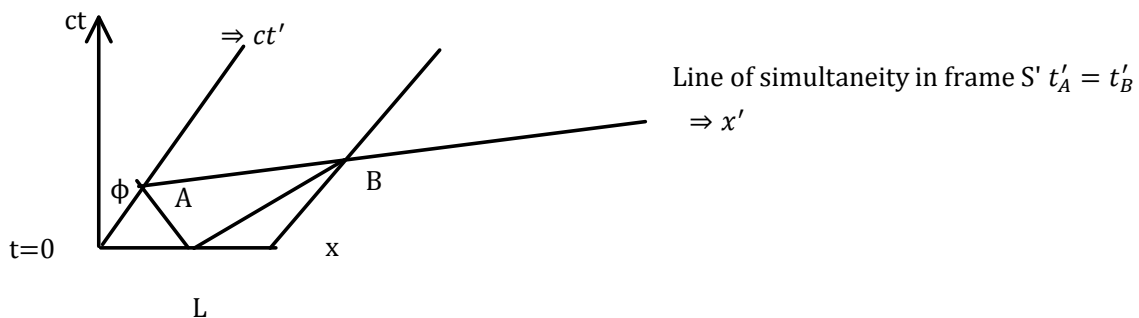
Send a light signal from the midpoint.

this reaches the ends of the rod at the same time (measured in the rest frame of the rod)

$$\Rightarrow t_A = t_B$$



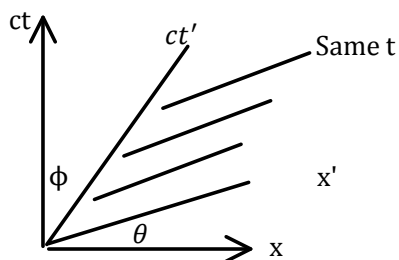
Now suppose rod is moving, with velocity  $v$   
Frame  $S'$  is co-moving with the rod



In moving frame  $S'$ , events A and B are considered simultaneous

Nb: uses both postulates of SR

1. Allows us to use same experimental definition of simultaneity
2.  $\Rightarrow$  speed of light is same in all frames



This is why we use skew axes  $(ct', x')$  in frame  $S'$   
Prove  $\theta = \phi$

$$\begin{aligned}
 x_A &= vt_A \\
 &= \frac{L}{2} - ct_A \Rightarrow ct_A = \frac{L}{2} \left( \frac{1}{1 + \frac{v}{c}} \right) \\
 x_B &= L + vt_B \\
 &= \frac{L}{2} + ct_B \Rightarrow ct_B = \frac{L}{2} \left( \frac{1}{1 - \frac{v}{c}} \right)
 \end{aligned}
 \tag{2}$$

$$\Rightarrow x_B - x_A = ct_B + ct_A \tag{1}$$

Obviously,  $t_A \neq t_B$

However, by definition  $t'_A = t'_B$

Angles

$$\begin{aligned}
 \tan \phi &= \frac{x_A}{ct_A} = \frac{v}{c} \\
 \tan \theta &= \frac{ct_B - ct_A}{x_B - x_A} = \frac{ct_B - ct_A}{ct_B + ct_A} \\
 &\quad \text{Using (1)} \\
 &= \frac{t_B - t_A}{t_B + t_A} \\
 &= \frac{1 + \frac{v}{c} - \left(1 - \frac{v}{c}\right)}{1 + \frac{v}{c} + \left(1 - \frac{v}{c}\right)} \\
 &\quad \text{Using (2)} \\
 &= \frac{v}{c}
 \end{aligned}$$

Check using Lorentz transformations

$$ct' = \gamma \left( ct - \frac{v}{c}x \right)$$

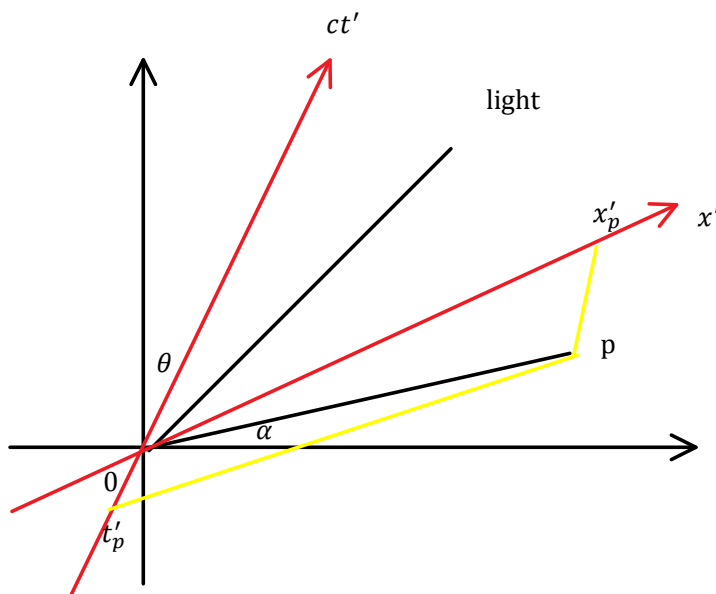
$$x' = \gamma \left( x - \frac{v}{c}ct \right)$$

$$x' \text{ axis is } t' = 0 \Rightarrow ct - \frac{v}{c}x = 0 \Rightarrow \tan \theta = \frac{ct}{x} = \frac{v}{c}$$

$$t' \text{ axis is } x' = 0 \Rightarrow x - \frac{v}{c}ct = 0 \Rightarrow \tan \phi = \frac{x}{ct} = \frac{v}{c}$$

### 3.2 faster than light/backwards in time

Suppose there exists a particle that can travel faster than light (Tachyon)



Op is a faster than light path

In frame S, op is forwards in time  $t_p > t_0$

In frame S', 0P is backwards in time,  $t'_p < t'_0$

$\Rightarrow$  If a faster than light signal is possible, Then in some frames it is forwards in time, but in other frames it is backwards in time

$$\tan \theta = \frac{v}{c}$$

$$\tan \alpha = \frac{c}{u}$$

Where  $u$  is the speed of the tachyon

Backwards in time in  $S'$  if the relativity velocity of the frames satisfies

$$\tan \theta > \tan \alpha$$

$$\Rightarrow \frac{v}{c} > \frac{c}{u} \Rightarrow v > \frac{c^2}{u}$$

Directly from Lorentz transformation

For  $0p$ ,

$$ct' = \gamma \left( ct - \frac{v}{c}x \right)$$

$$x' = \gamma \left( x - \frac{v}{c}ct \right)$$

Speed of tachyon  $u = \frac{x}{t}$

$$t' < 0 \text{ if } ct - \frac{v}{c}x < 0$$

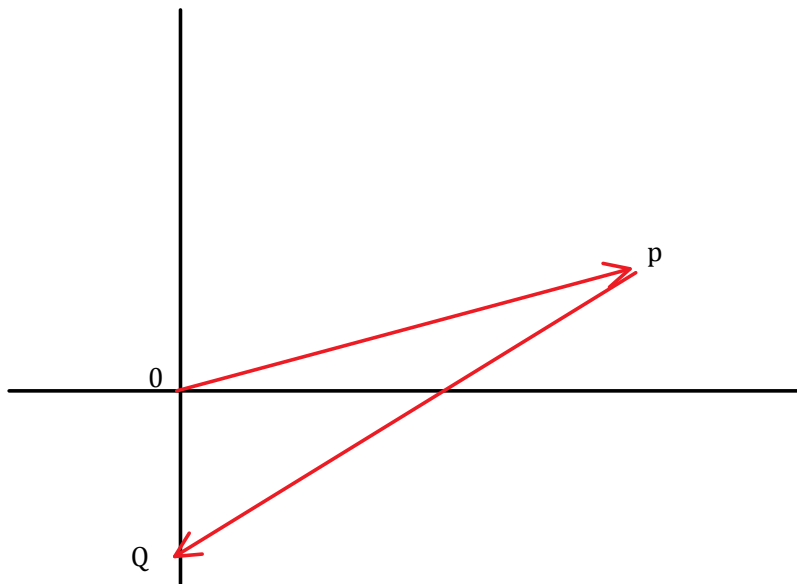
$$\Rightarrow ct \left( 1 - \frac{v}{c^2} \frac{x}{t} \right) < 0$$

$$\left( 1 - \frac{v}{c^2} \frac{x}{t} \right) \Rightarrow 1 - \frac{v}{c^2} u$$

$$\Rightarrow v > \frac{c^2}{u}$$

So far, this is not a terminal problem

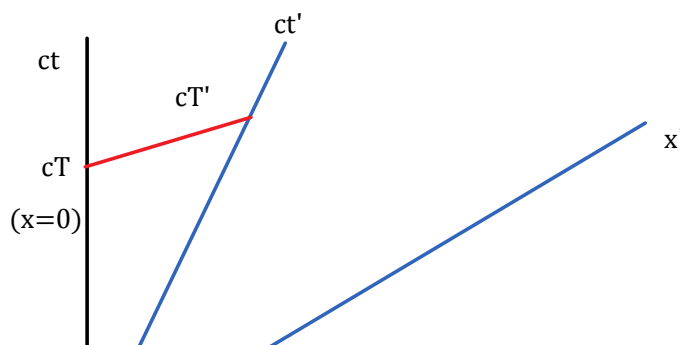
The problem is that once we accept faster than light/backwards in time in some frame is possible, Postulate I says that it is possible in all inertial frames in particular, it implies that if  $0p$  is possible, then so is motion  $PQ$

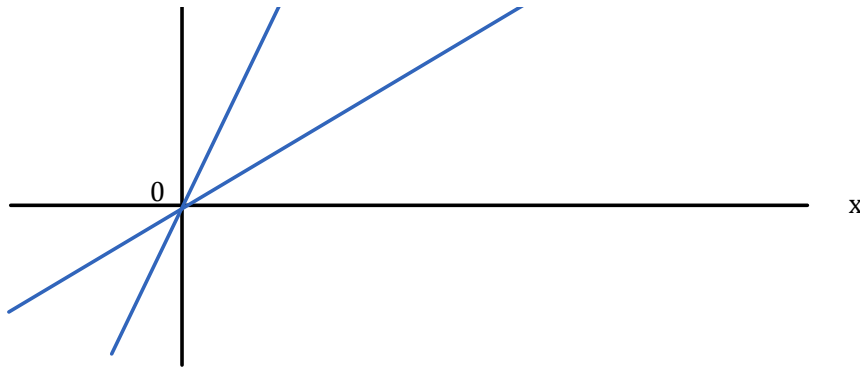


Closed path  $0PQ$  is incompatible with causality ("grandfather" paradox)

### 3.3 Time dilation

Measure time differences in frames  $S$  and  $S'$





In frame S, time interval is T  
 In frame S', time interval is T'  
 Where

$$T' = \gamma \left( T - \frac{vx}{c^2} \right) \Rightarrow \boxed{T' = \gamma T}$$

(since  $\frac{vx}{c^2} = 0$ )

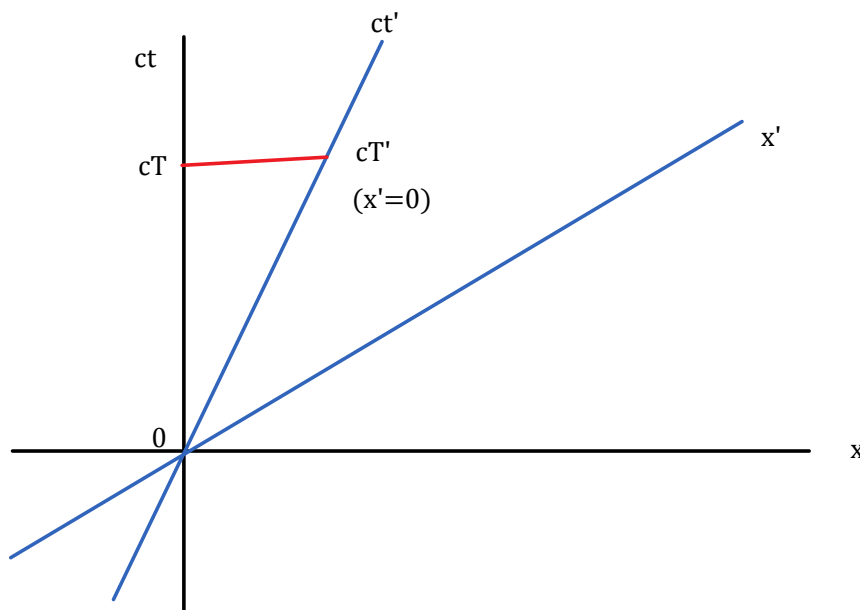
Remember

$$\gamma = \frac{1}{\sqrt{1 - \left(\frac{v^2}{c^2}\right)}} > 1$$

$$\Rightarrow T' > T$$

This is Time Dilation

Now, consider instead a time difference between the events in the same place in S'



Frame S', time interval = T'  
 Frame S, time interval = T  
 Where

$$T = \gamma \left( T' + \frac{v}{c^2} x \right)$$

$$\Rightarrow T = \gamma T'$$

So  $T > T'$

This must happen because postulate I says all inertial frames are the same  
 $\Rightarrow$  relation between measurements in S and S' must be symmetric

NB: this means that the minimum time between 2 events is the time measured in the frame where the events are at the same position

### 3.4 Length Contraction

Be very careful to be precise about what is being measured

#### 1. Space dilation

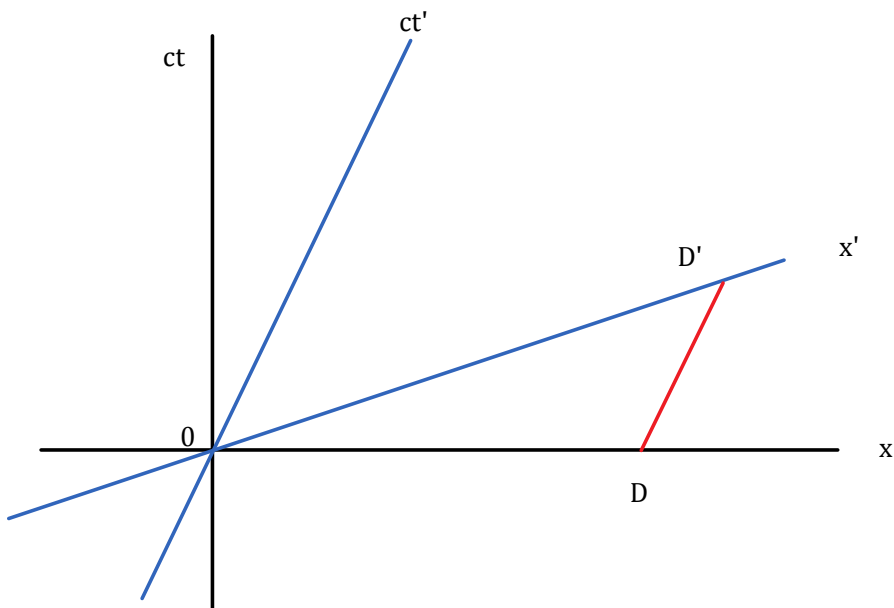
This is similar to time dilation

.

ct'

1. Space dilation

This is similar to time dilation



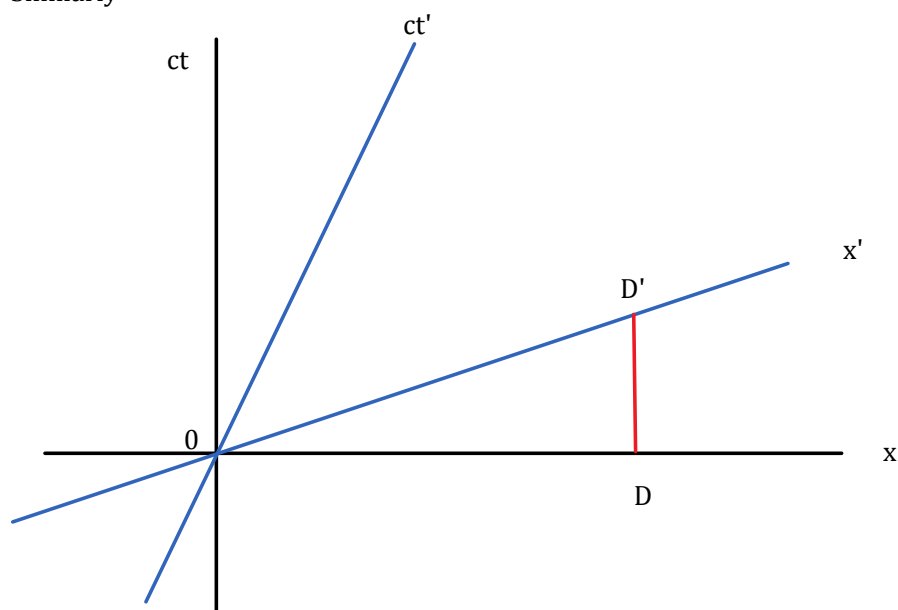
Frame S, distance = D

Frame S', distance = D'

Where

$$D' = \gamma \left( D - \frac{vt}{c^2} \right) = \gamma D$$

Similarly



Frame S', Distance = D'

(measured at same t')

Frame S, distance = D

$$D = \gamma \left( D' + \frac{vt'}{c^2} \right) = \gamma D' > D'$$

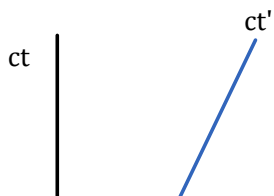
Length Contraction

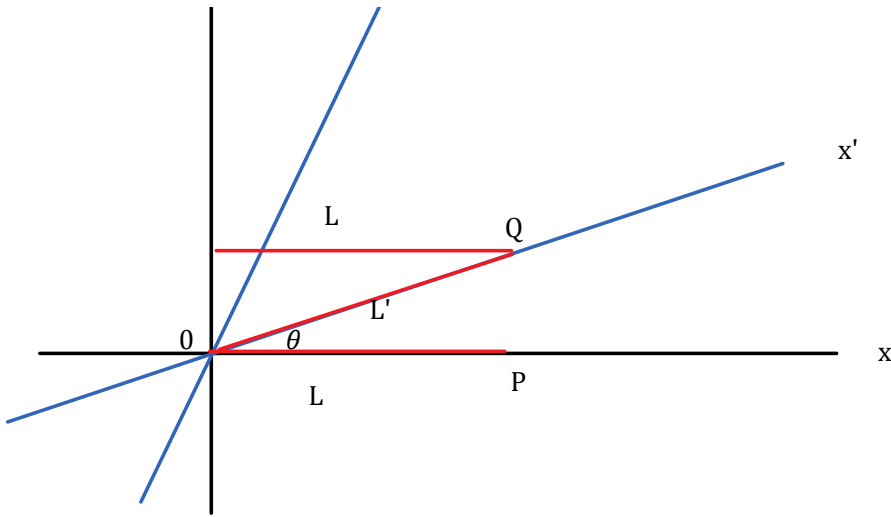
We need a definition of a measurement of length

Consider a rod of length L in frame S

Defn of length:

Length = distance between ends of rod measured AT THE SAME TIME





$\Rightarrow$  Length  $S$ ,  $L = x_P - x_0$

But in  $S'$ ,  $L' = x'_Q - x'_0$

So in frame  $S$ ,

$x_Q = L$

$ct_Q = L \tan \theta = L \frac{v}{c}$

$\Rightarrow$  in frame  $S'$

$x'_Q = \gamma(x_Q - vt_Q)$

$t'_Q = \gamma(t_Q - v \frac{x_Q}{c^2}) = 0$

$\Rightarrow L' = \gamma \left( L - \frac{v^2}{c^2} L \right)$

Since

$t'_Q = 0 \Rightarrow \frac{v}{c^2} x_Q$

$= \gamma \left( 1 - \frac{v^2}{c^2} \right) L$

$\Rightarrow \boxed{L' = \gamma^{-1} L}$

Since  $\gamma > 1, L' < L$

This is length contraction

Pole and garage "paradox"

Man carrying pole of length  $L'$  runs (fast) into a garage of length  $G$  garage is shorter than the pole,  $G < L'$

Paradox??

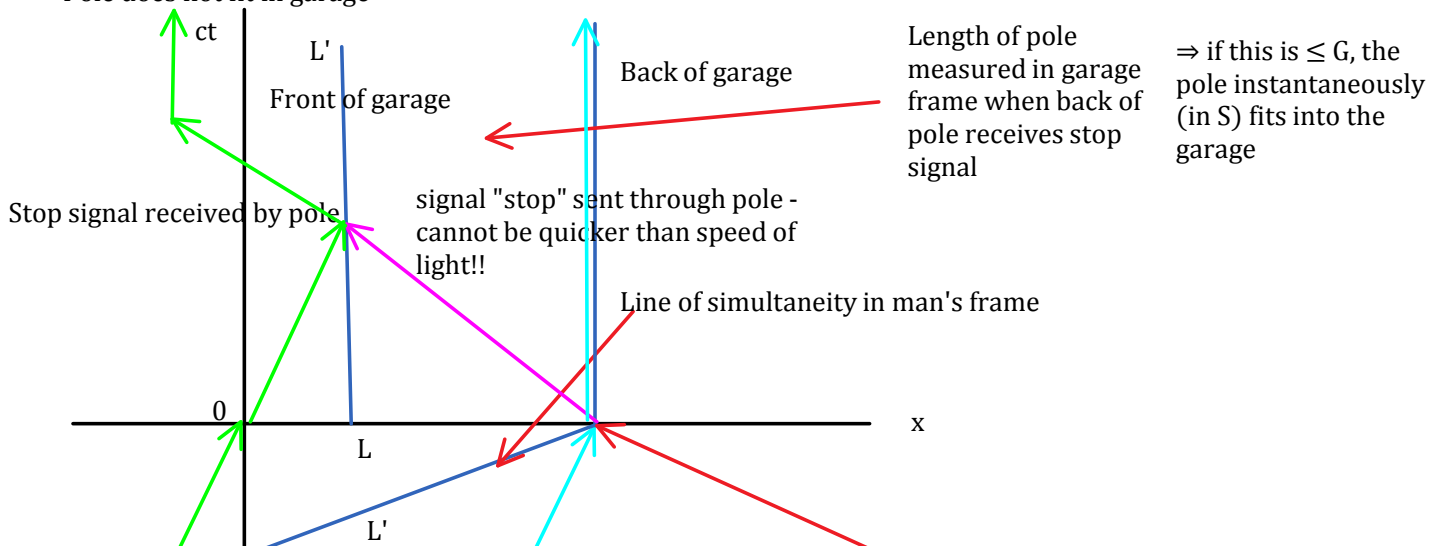
Garage frame- pole length is  $L = \gamma^{-1} L' < L'$

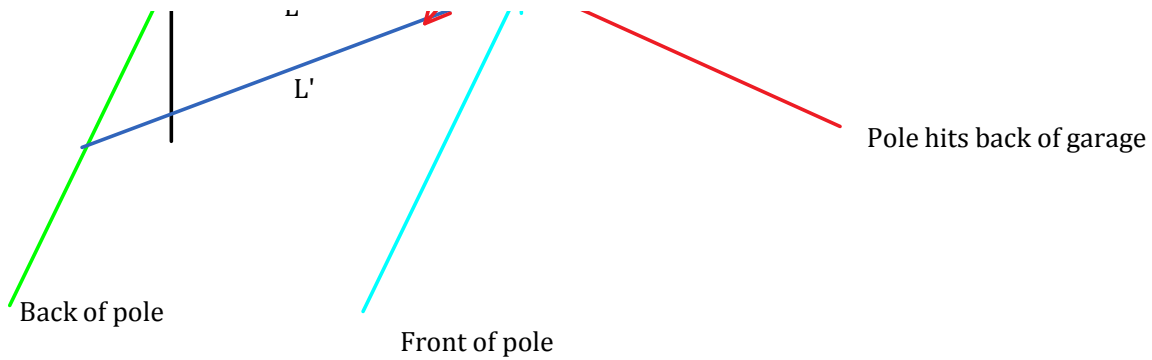
Can have  $L < G$

Pole fits inside the garage

Man's frame- garage is length contracted

$\Rightarrow$  Pole does not fit in garage





### Key points

Because signal speed is at most  $c$ , the back of the pole doesn't receive stop signal instantaneously, so keeps moving  $\Rightarrow$  pole is being physically compressed!

It is because the pole is being compressed that it can (for a moment) fit into the garage

Then it expands back to its normal length, and comes to rest outside the garage

NB

"rigid bodies" are incompatible with special relativity because signal speeds are always  $< c$

What is the max length of pole that fits into garage?

$$G = ct$$

$$L - G = vt$$

$$\Rightarrow L = \left(1 + \frac{v}{c}\right) G$$

But

$$L = \gamma^{-1} L'$$

$$\Rightarrow L' = \gamma \left(1 + \frac{v}{c}\right) G$$

$\uparrow$  longest pole that just fits into garage at speed  $v$

### 3.5 Velocity Addition Rule

Suppose a particle moves at velocity  $u$  in frame  $S$

What is its velocity  $u'$  in frame  $S'$ ?

$S'$  has velocity  $v$  relative to  $S$

In 1 dim

Lorentz transf

$$x' = \gamma(x - vt)$$

$$t' = \gamma\left(t - \frac{v}{c^2}x\right)$$

So for constant speed

$$u' = \frac{x'}{t'} = \frac{\gamma(x - vt)}{\gamma\left(t - \frac{v}{c^2}x\right)} = \frac{\gamma\left(\frac{x}{t} - v\right)}{\gamma\left(1 - \frac{v}{c^2}\frac{x}{t}\right)}$$

$$\Rightarrow u' = \frac{u - v}{1 - \frac{uv}{c^2}}$$

This replaces the newtonian result

$$u' = u - v$$

This is a good approximation in the limit where  $u, v$  are much less than  $c$

In 3dim

Let  $S'$  have velocity  $v$  along the  $x$  axis relative to  $S$

Lorentz transformation

$$x' = \gamma(x - vt)$$

$$y' = y$$

$$z' = z$$

$$t' = \gamma\left(t - \frac{v}{c^2}x\right)$$

$$\Rightarrow u'_x = \frac{u_x - v}{1 - \frac{u_x v}{c^2}}$$

$$u'_y = \frac{y'}{t'} = \frac{y}{\gamma\left(t - \frac{vx}{c^2}\right)} = \frac{uy}{\gamma\left(1 - \frac{u_x v}{c^2}\right)}$$

$$u'_z = \frac{uz}{\gamma \left(1 - \frac{u_x v}{c^2}\right)}$$

- This can be turned into the velocity addition formula  
Particle 1 moves with velocity  $u_1$  relative to the laboratory, and particle 2 moves with velocity  $u_2$  relative to particle 1  
 $\Rightarrow$ particle 2 speed in lab frame

$$\boxed{= \frac{u_1 + u_2}{1 + \frac{u_1 u_2}{c^2}}}$$

Conclude if  $u_1$  and  $u_2$  are both less than  $c$ , so is

$$\frac{u_1 + u_2}{1 + \frac{u_1 u_2}{c^2}}$$

- Consistency with postulate IB  
Speed of light is the same in all frames

$$\frac{u_1 - u_2}{1 - \frac{u_1 u_2}{c^2}}$$

If

$$u = c \Rightarrow u' = \frac{(c - v)}{1 - \frac{cv}{c^2}} = c$$

- From

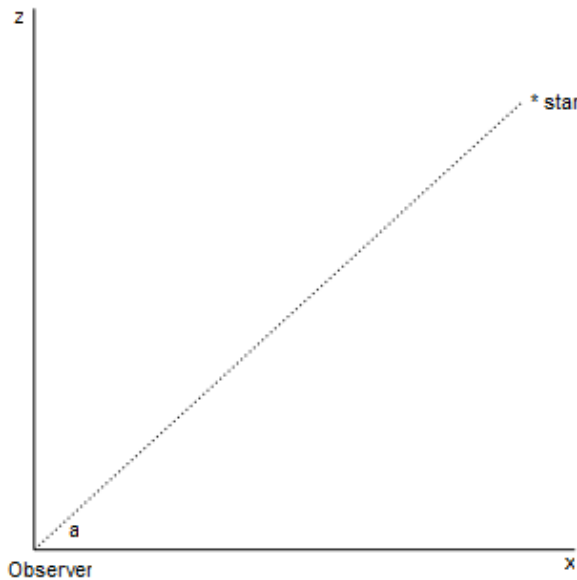
$$\frac{u - v}{1 - \frac{uv}{c^2}}$$

Same simple algebra shows that

$$\gamma(u') = \gamma(u)\gamma(v) \left(1 - \frac{uv}{c^2}\right)$$

### Stellar aberration

Apparent position of stars traces a small ellipse over the course of the earth's orbit around the sun  
This effect can be calculated accurately using the velocity addition formula

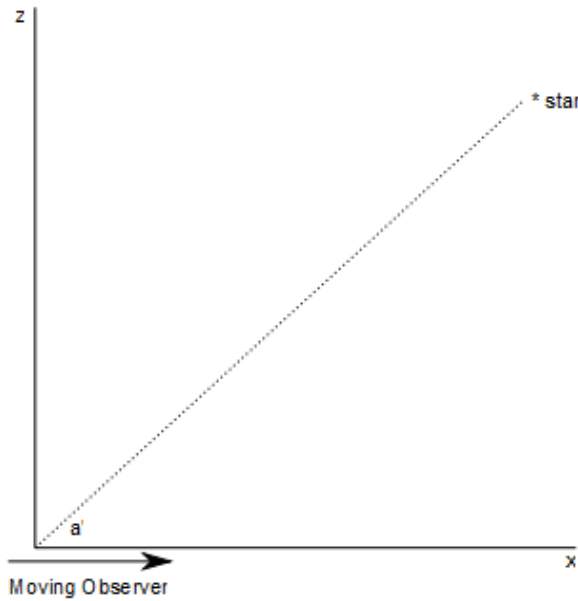


Suppose observer moves towards the star with velocity  $v$   
In moving frame

$$u'_x = \frac{u_x - v}{1 - \frac{u_x v}{c^2}} = -c \cos \alpha'$$

$$u'_z = \frac{u_z}{1 - \frac{u_z v}{c^2}} = -c \sin \alpha'$$





$$\Rightarrow \cos \alpha' = \frac{\cos \alpha + \frac{v}{c}}{1 + \frac{v}{c} \cos \alpha}$$

$$\sin \alpha' = \frac{\sin \alpha}{\gamma \left(1 + \frac{v}{c} \sin \alpha\right)}$$

We can tidy this up with a trig identity

$$\tan \frac{\alpha}{2} = \frac{\sin \alpha}{1 + \cos \alpha}$$

### 3.6 Doppler Effect

Frequency of light detected from a moving object is increased/decreased if the object is moving towards/away from the observer

This is the Doppler effect

In Newtonian dynamics, there are two different Doppler formulae depending on whether

- a. Source moves, detector stationary
- b. Detector moves, source stationary

In special relativity, only the relative motion of source and detector is real  $\Rightarrow$  there is only one Doppler formula that depends on the relative velocity

Consider a source moving with velocity  $v$  away from an observer (eg distant galaxy receding from earth)

Let the time at source between successive maxima of wave be  $dt_0 = \frac{1}{\nu_0}$ , where  $\nu_0$  = freq at source

The observer measures a time difference  $dt + \frac{v}{c} dt \rightarrow$  because source has moved

Where  $dt$  = time between wave maxima measured by observer

But special relativity (time dilation)  $\Rightarrow dt = \gamma dt_0$

So

$$dt_{obs} = dt + \frac{v}{c} dt = \gamma \left(1 + \frac{v}{c}\right) dt_0$$

$$\frac{\nu_{obs}}{\nu_0} = \frac{dt_0}{dt_{obs}} = \gamma^{-1} \left(1 + \frac{v}{c}\right)^{-1} = \frac{\sqrt{1 - \frac{v^2}{c^2}}}{1 + \frac{v}{c}}$$

time dilation gives extra factor  $\gamma$

$$\Rightarrow \frac{\nu_{obs}}{\nu_0} = \frac{\sqrt{1 - \frac{v}{c}}}{\sqrt{1 + \frac{v}{c}}}$$

Relativistic Doppler formula

$V$  +ve (source moving away)  $\Rightarrow \nu_{obs} < \nu_0$   
redshift

$V$  -'ve (source approaching)  $\Rightarrow v_0 < v_{obs}$

Blueshift

Transverse Doppler effect

In special relativity (only) there is a doppler effect even when the source is moving orthogonal to the direction of the signal

$$\frac{v_{obs}}{v_0} \Big|_{transverse} = \gamma^{-1}$$

## 4.1 Atomic Clocks and Time Dilation

07 November 2011

15:42

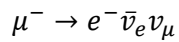
1971 Hafele & Keating fly atomic clocks around the world in opposite directions & compare  
SR  $\Rightarrow$  clocks following different paths so should register different times,

Clock going east: 59ns slow

West: 273 ns fast

### 4.2 Muon decay

Lifetime of a muon at rest is  $\sim 10^{-6}$  s



In 1966, CERN (small storage ring  $\sim 7$ m radius) with speeds  $0.997c$  ( $\Leftrightarrow \gamma = 12$ )

Lifetime was increased by a factor of 12

Time dilation

Repeated in 1978 with  $\gamma = 29$

For comparison, at LEP with energies 50GeV/beam  $\gamma$  factor is  $10^5$

# 5 Relativistic dynamics

14 November 2011

10:08

## 5.1 Vectors in Minkowski Spacetime

We formulate dynamics in special relativity using the language of 4-vectors

Prototype 4-vector is the position 4-vector,

$$x^\mu = (ct, \underline{x})$$

$$= (ct, x, y, z)$$

$$\mu = \begin{matrix} 0, & 1, & 2, & 3 \\ \text{time} & \text{space} & \text{space} & \text{space} \end{matrix}$$

Because it is a 4-vector,  $x^\mu$  transforms as

$$x'^\mu = L^\mu_\nu x^\nu$$

$$L^\mu_\nu = \begin{pmatrix} \gamma & -\gamma \frac{v}{c} & & \\ -\gamma \frac{v}{c} & \gamma & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$$

$$ct' = \gamma \left( ct - \frac{v}{c} x \right)$$

$$x' = \gamma \left( x - \frac{v}{c} ct \right)$$

$$y' = y$$

$$z' = z$$

ANY 4-vector has the same lorentz transformations

We can make a quantity out of  $x^\mu$  which is Lorentz invariant (doesn't change under a Lorentz transformation)

$$s^2 = g_{\mu\nu} x^\mu x^\nu = -c^2 t^2 + x^2 + y^2 + z^2 = -c^2 t^2 + \underline{x} * \underline{x}$$

$$g_{\mu\nu} = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$$

## 5.2 4-velocity

If we try to define the 4-velocity as

$$U^\mu = \frac{dx^\mu}{dt}$$

But this does NOT have the proper Lorentz transformation to be a 4-vector

To make a 4-vector we need to differentiate with respect to something which is itself Lorentz invariant.

$$S^2 = -c^2 t^2 + \underline{x} * \underline{x}$$

IS Lorentz invariant

Define the proper time  $\tau$ , where  $S^2 = -c^2 \tau^2$

$\tau$  is the actual time measured in a co-moving frame i.e. along the particles path

So define the velocity 4-vector as

$$U^\mu = \frac{dx^\mu}{d\tau}$$

So  $U^\mu$  has the correct Lorentz transformations

Components-

$$U^\mu = \frac{dx^\mu}{d\tau} = \frac{dt}{d\tau} \frac{dx^\mu}{dt}$$

Now

$$-c^2 \tau^2 = -c^2 t^2 + x^2 + y^2 + z^2 = -c^2 t^2 \left( 1 - \frac{x^2}{c^2 t^2} - \frac{y^2}{c^2 t^2} - \frac{z^2}{c^2 t^2} \right)$$

$$-c^2 \tau^2 \left( 1 - \frac{U_x^2}{c^2} - \frac{U_y^2}{c^2} - \frac{U_z^2}{c^2} \right)$$

$$\begin{aligned}
&= -c^2 t^2 \left(1 - \frac{u^2}{c^2}\right) \\
&= -c^2 t^2 \gamma^{-2}(U) \\
&\Rightarrow -c^2 \tau^2 = -c^2 t^2 \gamma^{-2}(u) \\
&\Rightarrow \tau = t \gamma^{-1}(u) \\
&\Rightarrow \boxed{\frac{dt}{d\tau} = \gamma(u)}
\end{aligned}$$

This implies that

$$\begin{aligned}
U^\mu &= \frac{dx^\mu}{d\tau} = \gamma(u) \frac{dx^\mu}{dt} \\
&\Rightarrow \boxed{U^\mu = (\gamma(u)x, \gamma(u)\underline{u})}, \text{ since } x^\mu = (ct, \underline{x})
\end{aligned}$$

Check Invariant

$$g_{\mu\nu} U^\mu U^\nu = -U^0 U^0 + U^1 U^1 + U^2 U^2 + U^3 U^3 = \gamma^2 (-c^2 + u^2) = -c^2$$

### 5.3 4-momentum and mass

The 4-momentum is defined as

$$P^\mu = m U^\mu$$

So the mass M is a Lorentz invariant quantity (!!)

$P^\mu$  has the correct Lorentz transformations to be a 4-vector

Its components are

$$\boxed{P^\mu = (\gamma(u)mc, \gamma(u)m\underline{u})}$$

The invariant formed from  $P^\mu$  is

$$g_{\mu\nu} P^\mu P^\nu = -\gamma^2 m^2 c^2 + \gamma^2 m^2 \underline{u} * \underline{u} = -m^2 c^2$$

So

$$P^2 \equiv g_{\mu\nu} P^\mu P^\nu = -m^2 c^2$$

That is, mass is the invariant quantity made from the 4-momentum (just like spacetime interval

$S^2$  made from the position 4-vector  $x^\mu$ )

Interpret components of the 4-momentum

Write

$$\begin{aligned}
P^\mu &= (P^0, \underline{p}) \\
\underline{p} &= \underline{3 - momentum}
\end{aligned}$$

$$\Rightarrow \boxed{\underline{p} = \gamma(u)m\underline{u}}$$

NB This is different from the usual Newtonian definition by the factor  $\gamma(u)$

The "timelike" component

$$P^0 = \gamma(u)mc = \left(1 - \frac{u^2}{c^2}\right)^{-\frac{1}{2}} mv$$

For small velocities  $u \ll c$ , expand

$$\gamma(u) = \left(1 - \frac{u^2}{c^2}\right)^{-\frac{1}{2}} = 1 + \frac{1}{2} \frac{u^2}{c^2} + O\left(\frac{u^4}{c^4}\right)$$

o=order?

$$\Rightarrow P^2 = 1 + \frac{1}{2} \frac{u^2}{c^2} + \dots$$

$$\leftrightarrow cP^2 = mc^2 + \frac{1}{2} mu^2$$

Notice that the newtonian kinetic energy is  $1/2 m$

This motivates use to identify  $cP^0$  as energy E

Thus

$$\begin{aligned}
P^\mu &= \left(\frac{E}{c}, \underline{p}\right) \\
E &= \gamma(u)mc^2 \\
\underline{p} &= \gamma(u)m\underline{u}
\end{aligned}$$

4-momentum

$$P^\mu = \left(\frac{E}{c}, \underline{p}\right)$$

Where

$$\underline{p} = \gamma(u)m\underline{u}$$

$$E = \gamma(u)mc^2$$

NB

(1) 3-momentum  $\underline{p}$  in special relativity is NOT  $\underline{p} = m\underline{u}$  but  $\boxed{\underline{p} = \gamma(u)m\underline{u}}$

For small velocities only ( $u \ll c$ ),  $\underline{p} \approx m\underline{u}$

(2) Identify  $\gamma(u)mc^2$  as energy E

For small  $u \ll c$

$$\gamma(u) = \left(1 - \frac{u^2}{c^2}\right)^{-\frac{1}{2}} \approx 1 + \frac{1}{2} \frac{u^2}{c^2} + \dots$$

$$\Rightarrow E = mc^2 + \frac{1}{2} mu^2 + \dots$$

$$\frac{1}{2} mu^2 \rightarrow \text{newtonian kinetic energy}$$

$$mc^2 \rightarrow \text{new in special relativity}$$

$$E \neq 0 \text{ even when particle is at rest}$$

Call this the "rest energy",

$$E_{rest} = mc^2$$

If the particle is moving

$$E = \gamma(u)mc^2$$

$E = mc^2$  opens the possibility of extracting energy from reactions where the total mass of constituents change

### Lorentz transformations

We already know the lorentz transformations for any 4-vector. They are exactly the same as for the position 4-vector

$$x^\mu = (ct, \underline{x})$$

Dictionary

$$x^\mu \leftrightarrow p^\mu$$

$$ct \leftrightarrow \frac{E}{c}$$

$$\underline{x} \leftrightarrow \underline{p}$$

$$g_{\mu\nu}u^\mu u^\nu \leftrightarrow g_{\mu\nu}p^\mu p^\nu$$

So we can immediately write the Lorentz transformations for energy and 3-momentum

$$p'^\mu = L^\mu_\nu p^\nu$$

$$\begin{cases} E' = \gamma(v)(E - vp_x) \\ P'_x = \gamma(v)\left(p_x - \frac{v}{c^2}E\right) \\ p'_y = p_y \\ p'_z = p_z \end{cases}$$

For a transformation between frames S and S' with relative velocity v in the x-direction

This shows that BOTH energy and momentum change when measured in different frames

As with any 4-vector, we can construct a Lorentz invariant quantity from  $p^\mu = \left(\frac{E}{c}, \underline{p}\right)$

Lorentz invariant is

$$g_{\mu\nu}p^\mu p^\nu$$

$$= -p^0 p^0 + p^1 p^1 + p^2 p^2 + p^3 p^3$$

$$= -\frac{E^2}{c^2} + p_x p_x + p_y p_y + p_z p_z$$

$$= -\frac{E^2}{c^2} + \underline{p} * \underline{p}$$

So the quantity

$$\left(-\frac{E^2}{c^2} + \underline{p} * \underline{p}\right)$$

Is invariant under Lorentz transformations

Evaluate

$$-\frac{E^2}{c^2} + \underline{p} * \underline{p} = -\gamma(u)^2 m^2 c^2 + \gamma(u)^2 m^2 u^2$$

$$= -\gamma^2(u) \left(1 - \frac{u^2}{c^2}\right) m^2 c^2 = -m^2 c^2$$

→ so the Lorentz invariant quantity is the mass

We find

$$E^2 - c^2 \underline{p} * \underline{p} = m^2 c^4$$

$$\boxed{E^2 - c^2 p^2 = m^2 c^4}$$

This holds for any frame

CHECK explicitly

$$E'^2 - c^2 p'^2 = m^2 c^4$$

Using Lorentz transformations

### Photons

Photons have zero mass

$$\Rightarrow E^2 - c^2 p^2 = 0$$

$$E = c|p|$$

Photon 4-momentum

$$p^\mu = \left(\frac{E}{c}, \underline{p}\right)$$

For a massive particle,  $p^\mu = (\gamma(u)mc, \gamma(u)m\underline{u})$

The formula for a photon is the singular limit

$$m \rightarrow 0, \gamma(u) \rightarrow \infty$$

$$\Rightarrow u \rightarrow c$$

This is a consequence of the fact that a massless particle (photon) must travel at the speed of light,  $u = c$

### 5.4 Postulates of relativistic dynamics

To complete the formulation of dynamics in special relativity, we give the analogues of Newton's laws

1a. Equivalence of all inertial frames (there aren't? global inertial frames)

1b. Speed of light is the same in all inertial frames

Introduces a new fundamental constant  $c$  into physics

2. This introduces the idea of a force 4-vector

$$F^\mu = \frac{dP^\mu}{d\tau}$$

$\tau$  = proper time

Generalises Newtonian

$$\underline{f} = \frac{d\underline{P}}{dt}$$

$$\Leftrightarrow F^\mu = \gamma(u) \left(\frac{1}{c} \frac{dE}{dt}, \frac{d\underline{P}}{dt}\right) = (F^0, \gamma(u)\underline{f})$$

So in particular

$$\underline{f} = \frac{d\underline{p}}{dt}$$

In S. Rel

3. Dynamics takes place in spacetime.

Laws of physics are invariant under translations in space and time

Noether's theorem  $\Rightarrow$  conservation of 3-momentum and energy

i.e. invariance under translations in spacetime  $\Rightarrow$  conservation of 4-momentum  $p^\mu$

In practice, to solve problems in relativistic dynamics, we use two main tools

1) Energy + 3 momentum conservation

2) Energy-momentum mass relation  $E^2 - c^2|\underline{p}|^2 = m^2 c^4$

Remembering mass  $m$  is Lorentz invariant

# 6 Relativistic collisions

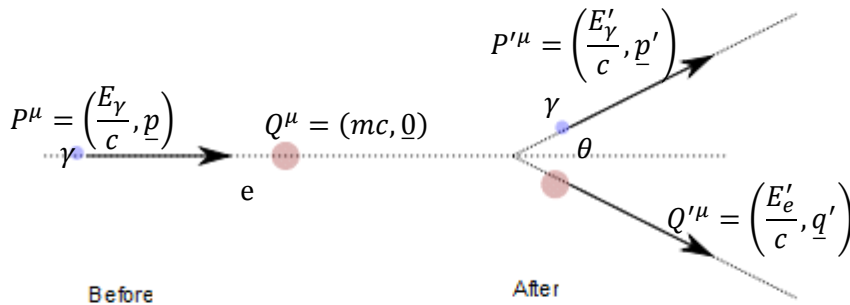
21 November 2011

10:25

## 6.1 Compton effect

Collision between a photon and electron, in which the electron is initially at rest  
 After collision, photon loses energy  $\Rightarrow$  wavelength increases (red shifted)

1922, Compton, using x-rays



Let

$$P^\mu = \left(\frac{1}{c}E_\gamma, \underline{p}\right)$$

$$Q^\mu = (mc, \underline{0})$$

$$mc = \frac{1}{c}E_e$$

$$\underline{q} = \underline{0}$$

And

$$P'^\mu = \left(\frac{1}{c}E'_\gamma, \underline{p}'\right)$$

$$Q'^\mu = \left(\frac{1}{c}E'_e, \underline{q}'\right)$$

Use energy and momentum conservation separately

$$E'_e = E_e + E_\gamma - E'_\gamma$$

$$\underline{q}' = \underline{q} + \underline{p} - \underline{p}'$$

Energy-momentum-mass relation for photons

$$E_\gamma = c|\underline{p}|$$

$$E'_\gamma = c|\underline{p}'|$$

Energy-momentum-mass relation for electron

$$E_e'^2 - c^2|\underline{q}'|^2 = m^2c^4$$

But

$$E_e'^2 - c^2|\underline{q}'|^2 = (mc^2 + c|\underline{p}| - c|\underline{p}'|)^2 - c^2(|\underline{p}|^2 + |\underline{p}'|^2 - 2|\underline{p}||\underline{p}'|\cos\theta)$$

$$= m^2c^4 + 2mc^3(|\underline{p}| - |\underline{p}'|) + c^2(|\underline{p}| - |\underline{p}'|)^2 - c^2|\underline{p}|^2 - c^2|\underline{p}'|^2 + 2c^2|\underline{p}||\underline{p}'|\cos\theta$$

$$= m^2c^4 + 2mc^3(|\underline{p}| - |\underline{p}'|) - 2c^2|\underline{p}||\underline{p}'|(1 - \cos\theta)$$

Conclude

$$\boxed{mc(|\underline{p}| - |\underline{p}'|) = |\underline{p}||\underline{p}'|(1 - \cos\theta)}$$



Or,

$$E_\gamma - E'_\gamma = \frac{1}{mc^2} E_\gamma E'_\gamma (1 - \cos \theta)$$

So energy of scattered photon  $E'_\gamma$  depends on the scattering angle  $\theta$

Bigger scattering angle  $\Leftrightarrow$  bigger energy loss

In quantum mechanics

$$E_\gamma = h\nu = \frac{hc}{\lambda}$$

$$\Rightarrow \lambda' - \lambda = \frac{h}{mc} (1 - \cos \theta)$$

$$E_\gamma E'_\gamma (1 - \cos \theta) = mc(E_\gamma - E'_\gamma)$$

$\theta \approx 0$  small angle scattering  $E'_\gamma \approx E_\gamma$

$\hat{\theta}$  bigger  $\Leftrightarrow$  Bigger energy loss,  $E'_\gamma \ll E_\gamma$

This is "normal" Compton scattering, i.e. where the photon loses energy

"Inverse" Compton scattering is where the photon is back-scattered from a high-energy electron and gains energy.

This is important

- 1) Lab, to get high-energy photon beam
- 2) Astrophysics, i.e. gamma-ray burst

### Compton scattering with 4-momentum notation

Notation

$$P \cdot Q = g_{\mu\nu} P^\mu Q^\nu = -P^0 Q^0 + P^1 Q^1 + P^2 Q^2 + P^3 Q^3$$

$$g_{\mu\nu} = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$$

$$g_{\mu\nu} P^\mu Q^\nu = P^\mu g_{\mu\nu} Q^\nu = (1 * 4)(4 * 4)(4 * 1)$$

$$= 1 * 1 = \text{number}$$

$$P^2 = g_{\mu\nu} P^\mu P^\nu$$

So, e.g.

$$Q' = \left( \frac{E'_e}{c}, \underline{q}' \right)$$

$$Q'^2 = \frac{1}{c^2} E_e'^2 + \underline{q}' \cdot \underline{q}'$$

$$= -m^2 c^2$$

Similarly

$$P = \left( \frac{E_\gamma}{c}, \underline{p} \right)$$

$$P^2 = -\frac{E_\gamma^2}{c^2} + \underline{p} \cdot \underline{p}$$

So, using energy-momentum conservation in Compton scattering

$$P^\mu + Q^\mu = P'^\mu + Q'^\mu$$

$$\Rightarrow Q'^\mu = Q^\mu + P^\mu - P'^\mu$$

So, using the energy-momentum-mass relation

$$Q'^2 = Q^2 + 2Q \cdot (P - P') + P^2 + P'^2 - 2P \cdot P'$$

$$Q'^2 = -m^2 c^2$$

$$Q^2 = -m^2 c^2$$

$$P^2 = P'^2 = 0$$

$$Q \cdot (P - P') = P \cdot P'$$

$$-mc \left( \frac{1}{c} E_\gamma - \frac{1}{c} E'_\gamma \right) =$$

Since

$$P \cdot P' = -\frac{E_\gamma E'_\gamma}{c^2} + \underline{P} \cdot \underline{P}' = -\frac{E_\gamma E'_\gamma}{c^2} + |\underline{P}| |\underline{P}'| \cos \theta$$

$$= -\frac{E_\gamma E'_\gamma}{c^2} (1 - \cos \theta)$$

$$E_\gamma E'_\gamma (1 - \cos \theta) = mc^2 (E_\gamma - E'_\gamma)$$

Reproducing the results already found

NB equivalence between these steps and those in the original derivation

## 6.2 Colliding Beams

Modern particle fall into two categories- colliders and fixed target

In a collider, 2 beams are accelerated and stored in counter-rotating rings, then collided head-on

Examples

LHC	P P	3.5 TeV beams
LEP	$e^+ e^-$	50-100GeV
$Spp\bar{p}S$	$p\bar{p}$	270GeV
		CERN
HERA	$e^- p$	
		DESY

+lots of other lower-energy  $e^+ e^-$

CERN

ISR,

Pp

Few GeV

In a fixed target accelerator, a high-energy beam of particles is scattered from a stationary target

CERN: SPS p beam  $\rightarrow$   $\square$

270GeV beam

(super proton synchrotron)

Original PS  $\sim$  27GeV

## 6.2 Colliding beams (cont.)

The simplest example of a particle collider is LEP, which collided beams of  $e^+$  and  $e^-$  with equal energies, initially  $E_{beam} \approx 50\text{GeV}$

Two electrons

$$P_2^\mu = \left( \frac{E}{c}, -\underline{p} \right)$$

$$P_1^\mu = \left( \frac{E}{c}, \underline{p} \right)$$

$$E = E_{beam}$$

Energy-momentum-mass relation

$$\text{Recall } P^2 = g_{\mu\nu} P^\mu P^\nu$$

$$= -P^0 P^0 + \underline{P} \cdot \underline{P} = -\frac{E^2}{c^2} + |\underline{P}|^2$$

$$P_1^2 = -\frac{E^2}{c^2} + |\underline{P}|^2 = -m^2 c^2$$

$$P_2^2 = -\frac{E^2}{c^2} + |\underline{P}|^2 = -m^2 c^2$$

Total 4-momentum

$$P_T^\mu = P_1^\mu + P_2^\mu = \left( \frac{2E}{c}, \underline{0} \right)$$

This is in the lab frame. In this special case (only), this is also the Centre of Momentum (CM) frame

In general, the CM frame is defined as the frame of reference where the total 3-momentum is zero.

We can always find this frame by making an appropriate Lorentz transformation.

In the CM frame, the total energy  $E_T^{CM}$  is available to make new particles eg at LEP,  $e^+e^- \rightarrow Z$

So at LEP

$$E_T^{CM} = E_T^{lab} \\ = 2 \times 50 = 100 \text{ GeV}$$

Maximum mass of new particle is

$$m = \frac{2E}{c^2}$$

Not all colliders are symmetric

Eg at DESY, the  $e^-p$  collider HERA collided beams of  $e^-$  with energy 26 GeV and with energy 840 GeV

Electron 4-momentum

$$P_1^\mu = \left( \frac{E_1}{c}, \underline{P}_1 \right)$$

Proton 4-momentum

$$P_2^\mu = \left( \frac{E_2}{c}, \underline{P}_2 \right)$$

Energy-momentum-mass relations,

$$P_1^2 = -\frac{E_1^2}{c^2} + |\underline{P}_1|^2 = -m_1^2 c^2 \\ m_1 = \text{electron mass} \approx 0.5 \text{ MeV}$$

$$P_2^2 = -\frac{E_2^2}{c^2} + |\underline{P}_2|^2 = -m_2^2 c^2 \\ m_2 = \text{proton mass} \approx 1 \text{ GeV}$$

Total 4-momentum in LAB frame

$$P_T^\mu = \left( \frac{E_1 + E_2}{c}, \underline{P}_1 + \underline{P}_2 \right)$$

By definition, in CM frame

$$P_{T CM}^\mu = \left( \frac{E_1 + E_2}{c}, \underline{0} \right) = \left( \frac{E_{CM}}{c}, \underline{0} \right)$$

Problem is to find  $E_{CM}$

2 ways

- 1) Explicitly work out the velocity  $v$  of the CM frame  $S'$  relative to LAB frame  $S$ , so that  $\underline{P}'_1 + \underline{P}'_2 = 0$  then calculate  $E'_1 + E'_2$ , using Lorentz transformation. -usually relatively hard
- 2) The quantity  $P_T^2 = -g_{\mu\nu} P_T^\mu P_T^\nu$  is Lorentz invariant, so is the same whether we evaluate in LAB frame  $S$  or the CM frame  $S'$

LAB frame

$$P_T^2 = -\left( \frac{E_1 + E_2}{c} \right)^2 + (\underline{P}_1 + \underline{P}_2) \cdot (\underline{P}_1 + \underline{P}_2) \\ = -\frac{E_1^2}{c^2} - \frac{E_2^2}{c^2} - 2E_1 E_2 + |\underline{P}_1|^2 + |\underline{P}_2|^2 + 2\underline{P}_1 \cdot \underline{P}_2 \\ = -m_1^2 c^2 - m_2^2 c^2 - \frac{2E_1 E_2}{c^2} - 2|\underline{P}_1||\underline{P}_2|$$

By definition, in CM frame

$$= \left( \frac{E_1 + E_2}{c}, \underline{0} \right) \cdot \left( \frac{E_{CM}}{c}, \underline{0} \right)$$

CM frame

$$P_{T CM}^\mu = -\frac{E_{CM}^2}{c^2}$$

Since

$$P_{T CM}^2 = m_1^2 c^4 + m_2^2 c^4 + 2E_1 E_2 + 2|\underline{P}_1||\underline{P}_2| c^2$$

In general, this is the final result. (remembering  $|\underline{P}_1|$  and  $|\underline{P}_2|$  are given in terms of energies  $E_1$  and  $E_2$  by  $-\frac{E_i^2}{c^2} + |\underline{P}_i|^2 = -m_i^2 c^2$  etc)

In practice, eg at HERA, masses are small compared to beam energies

Since

$$m_1 c^2 \ll E_1, m_2 c^2 \ll E_2, \text{ we can neglect } m_1, m_2 \text{ and } c|\underline{P}_1| \approx E_1, c|\underline{P}_2| \approx E_2$$

So to an excellent approximation

$$E_{CM}^2 \approx 4E_1 E_2 \Rightarrow \boxed{E_{CM} \approx 2\sqrt{E_1 E_2}}$$

This is the general result for an asymmetric, high-energy collider where  $E_{beam} \gg mass$

Clearly, in the special case of equal energy-beams,  $E_1 = E_2 = E_{beam}$   
 $\Rightarrow E_{CM} = 2E_{beam}$  as for LEP

### 6.3 Fixed target accelerators

Eg SPS (super-proton-synchrotron) at CERN

Proton beam  $E_{beam} = 270 GeV$

Collides with a fixed proton target

$$P_1^\mu = \left( \frac{E}{c}, \underline{P} \right)$$

Accelerated proton

$$P_2^\mu = (Mc, \underline{0})$$

Rest proton,  $m = \text{mass of proton}$

$$\Rightarrow P_T^\mu = P_1^\mu + P_2^\mu = \left( \frac{E + Mc^2}{c}, \underline{P} \right)$$

In CM frame, by definition,

$$P_{T\ CM}^\mu = \left( \frac{E_{CM}}{c}, \underline{0} \right)$$

Lorentz invariant

$$P_{T\ CM}^2 = P_{T\ LAB}^2$$

Now,

$$P_{T\ CM}^2 = -\frac{E_{CM}^2}{c^2}$$

$$P_{T\ LAB}^2 = -\frac{(E + Mc^2)^2}{c^2} + |\underline{P}|^2$$

$$= -\frac{E^2}{c^2} + |\underline{P}|^2 - 2EM - M^2 c^2$$

$$-\frac{E^2}{c^2} + |\underline{P}|^2 = -M^2 c^2$$

$$= -2EM - 2M^2 c^2$$

So we find

$$E_{CM}^2 = 2EMc^2 + 2M^2 c^4$$

For high energy accelerators,  $E_{beam} \gg Mc^2$

So an excellent approximation is

$$E_{CM}^2 \approx 2EMc^2$$

$$\Rightarrow \boxed{E_{CM} \approx \sqrt{2EMc^2}}$$

Compare collider

$$E_{CM} \approx 2\sqrt{E_1 E_2}$$

So for a given beam energy,  $E_{CM}$  is much bigger for a collider

Energy conservation

$$E_1 + mc^2 = E_2 + E_3$$

3-momentum conservation

$$\underline{P}_1 = \underline{P}_3 + \underline{P}_4$$

Where  $\theta = \theta_3 + \theta_4$

$$\Rightarrow |\underline{P}_1|^2 = |\underline{P}_3|^2 + |\underline{P}_4|^2 + 2|\underline{P}_3||\underline{P}_4| \cos \theta$$

Consider a special case where the particles separate with equal energies

Assume  $E_3 = E_4$

$$\Rightarrow \underline{P}_3 = \underline{P}_4$$

$$\Rightarrow \theta_3 = \theta_4$$

By conservation of transverse momentum

So the conservation equations simplify

$$E_1 + mc^2 = 2E_3$$

$$E_1^2 - m^2c^4 = 2(E_3^2 - m^2c^4)(1 + \cos \theta)$$

Using  $E_1^2 - c^2|p_1|^2 = m^2c^4$  etc

Now solve these to find scattering angle  $\theta$  as a function of the initial beam energy  $E_1$

Algebra,

$$1 \Rightarrow E_1^2 - m^2c^4 = (E_1 + mc^2)(E_1 - mc^2) = 4E_3(E_3 - mc^2)$$

Compare 1 and 2

$$\Rightarrow 4E_3(E_3 - mc^2) = 2(E_3^2 - m^2c^4)(1 + \cos \theta) = 2(E_3 + mc^2)(E_3 - mc^2)(1 + \cos \theta)$$

$$\Rightarrow 1 + \cos \theta = \frac{4E_3}{2(E_3 + mc^2)}$$

$$\Rightarrow \cos \theta = \frac{E_3 - mc^2}{E_3 + mc^2}$$

Finally, substitute for  $E_3$  using  $2E_3 = E_1 + mc^2$

$$\Rightarrow \cos \theta = \frac{E_1 - mc^2}{E_1 + 3mc^2}$$

At low energies,  $E_1 \approx mc^2$

$$\Rightarrow \cos \theta \approx 0 \Leftrightarrow \theta \approx 90^\circ$$

So the particles scatter at right angles

this is the well known result in Newtonian dynamics (snooker without spin)

At high energies,  $E_1 \gg mc^2$

$$\Rightarrow \cos \theta \approx 1 \Leftrightarrow \theta \approx 0$$

The higher the energy, the smaller the scattering angle. The particles are scattered into a narrow forward cone. This is a very general result in relativistic scattering.

### 2+2 scattering in the CM frame

The analysis above was for the lab frame. Now recover the same result in the CM frame

~~

Momenta are equal and opposite in x-direction

Suppose the relative velocity of the CM frame and lab frame is  $v$

$$\Rightarrow E_2^{CM} = \gamma(v)m$$

Now we showed previously that the total CM energy for fixed-target scattering is

$$E_{CM} = \sqrt{2m(E + m)}$$

$$E_1^{CM} = \frac{1}{2}\sqrt{2m(E + m)}$$

And since  $E_1^{CM} = \gamma(v)m$

$$\Rightarrow \gamma(v) = \frac{1}{2m}\sqrt{2m(E + m)}$$

$$\Rightarrow \sqrt{\frac{E + m}{2m}}$$

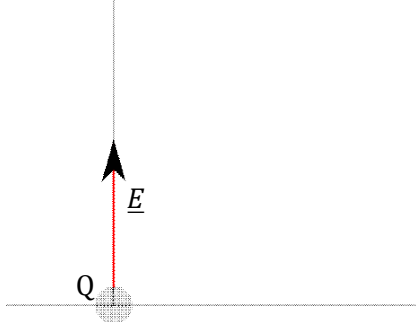
This determines the velocity  $v$  at the CM frame relative to the LAB frame

# 7 Electromagnetism

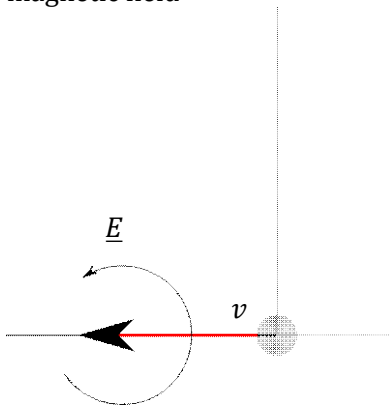
05 December 2011

10:20

A charge at rest in frame S has only an electric field.



But in frame S' (moving with velocity v in x-direction), this will appear to be a current  $\Rightarrow$  in S' there will also be a magnetic field



Electric & magnetic fields transform into each other as we change frames

Lorentz transformations

$$E'_x = E_x; E'_y = \gamma(v)(E_y - vB_z); E'_z = \gamma(v)(E_z + vB_y)$$

$$B'_x = B_x; B'_y = \gamma(v)\left(B_y + \frac{v}{c^2}E_z\right); B'_z = \gamma(v)\left(B_z + \frac{v}{c^2}E_y\right)$$

Identify  $\underline{E}$  and  $\underline{B}$  fields by their effect on a test charge q given by Lorentz force  $\underline{f} = q(\underline{E} + \underline{u} \times \underline{B})$

$\underline{u}$  = Velocity of charge q

Since we know how force transforms between S and S', we can use the Lorentz force law to deduce the transformation of  $\underline{E}$  and  $\underline{B}$

## 7.1 Lorentz transformations for force

These are implicit in section 5 where we write the Lorentz transformations for the 4-force  $F^\mu$

Explicitly:-

$$\underline{f} = \frac{d}{dt}\underline{p} \Rightarrow f' = \frac{d}{dt'}\underline{p}' = \left(\frac{dt'}{dt}\right)^{-1} \frac{d}{dt}\underline{p}'$$

$$p'_x = \gamma(v)\left(p_x - \frac{vE}{c^2}\right)$$

$$p'_y = p_y$$

$$p'_z = p_z$$

$$\Rightarrow \frac{d}{dt}p'_x = \gamma(v)\left(\frac{dp_x}{dt} - \frac{v}{c^2}\frac{dE}{dt}\right)$$

$$\frac{d}{dt}p'_y = \frac{d}{dt}p_y$$

Calculate  $\frac{dE}{dt}$ : -

$$E^2 = c^2 \underline{p} \cdot \underline{p} + m^2 c^4$$

$$\Rightarrow 2E \frac{dE}{dt} = 2c^2 \underline{p} \cdot \frac{d\underline{p}}{dt}$$

$$\Rightarrow \frac{dE}{dt} = \frac{c^2 \underline{p}}{E} \cdot \frac{d\underline{p}}{dt} - \underline{u} \cdot \frac{d\underline{p}}{dt}$$

But

$$E = \gamma(u) m c^2$$

$$\underline{p} = \gamma(v) m \underline{u}$$

So

$$f'_x = \left( \frac{dt'}{dt} \right)^{-1} \gamma(v) \left( \frac{dp_x}{dt} - \frac{v}{c^2} \underline{u} \cdot \frac{d\underline{p}}{dt} \right)$$

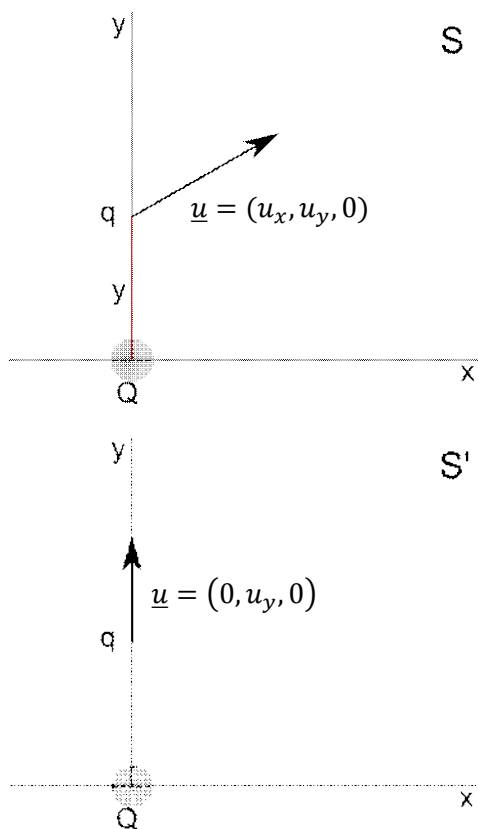
$$= \frac{1}{\gamma(v) \left( 1 - \frac{u_x v}{c^2} \right)} \gamma(v) \left( f_x - \frac{v}{c^2} \underline{u} \cdot \underline{f} \right)$$

$$f'_x = \frac{1}{\left( 1 - \frac{u_x v}{c^2} \right)} \left( f_x - \frac{v}{c^2} \underline{u} \cdot \underline{f} \right)$$

$$f'_y = \frac{1}{\left( 1 - \frac{u_x v}{c^2} \right)} f_y, \text{ sim for } f'_z$$

## 7.2 Electric and magnetic fields

Consider a simple configuration of a charge Q with a test charge q



S' moving with velocity v w.r.t. S

In frame S, the force experienced by the test charge is

$$\underline{f} = (0, f_y, 0)$$

Where

$$f_y = q\epsilon, \epsilon = \frac{1}{4\pi\epsilon_0} \frac{Q}{y^2}$$

In frame S', the force is

$$f'_x = \frac{1}{\left(1 - \frac{u_x v}{c^2}\right)} \left( f_x - \frac{v}{c^2} \underline{u} \cdot \underline{f} \right)$$

$$= \frac{1}{\left(1 - \frac{u_x v}{c^2}\right)} \left( f_x - \frac{v}{c^2} v f_x - \frac{v}{c^2} u_y f_y \right) = -\gamma(v)^2 \frac{v u_y}{c^2} q \epsilon$$

$$= -\gamma(v) \frac{v u'_y}{c^2} q \epsilon$$

$$f'_y = \frac{1}{\left(1 - \frac{u_x v}{c^2}\right)} f_y = \gamma(v) q \epsilon$$

$$f'_z = 0$$

Now use the Lorentz force law to deduce  $\underline{E}'$  and  $\underline{B}'$  fields

$$\Rightarrow \underline{E}' = (0, \gamma(v)\epsilon, 0), \underline{B}' = \left(0, 0, -\gamma(v) \frac{v}{c^2} \epsilon\right)$$

In frame S'

$$\text{Since } \underline{f}' = q(\underline{E}' + \underline{u}' \times \underline{B}')$$

Compare

$$\underline{E} = (0, \epsilon, 0), \underline{B} = (0, 0, 0)$$

In frame S

Check that the special case agrees with the general lorentz transformations for E and B given above

### 7.3 Electromagnetic field tensor

We have justified the following lorentz transformations for components of the electric & magnetic field vectors

$$E'_x = E_x \quad E'_y = \gamma(v)(E_y - v B_z) \quad E'_z = \gamma(v)(E_z + v B_y)$$

$$B'_x = B_x \quad B'_y = \gamma(v)\left(B_y + \frac{v}{c^2} E_z\right) \quad B'_z = \gamma(v)\left(B_z - \frac{v}{c^2} E_y\right)$$

We would like to describe these in the same way as for 4-vector eg

$$x' = Lx \Leftrightarrow x'^{\mu} = L^{\mu}_{\nu} x^{\nu}$$

$$P' = LP \Leftrightarrow P'^{\mu} = L^{\mu}_{\nu} P^{\nu}$$

Where

$$L^{\mu}_{\nu} = \begin{pmatrix} \gamma & -\frac{\gamma v}{c} & & \\ -\frac{\gamma v}{c} & \gamma & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$$

To incorporate the 6 components of  $\underline{E}$  and  $\underline{B}$ , put them into an antisymmetric 4\*4 matrix  $F^{\mu\nu}$

$$F^{\mu\nu} = \begin{pmatrix} & -\frac{1}{c} E_x & -\frac{1}{c} E_y & -\frac{1}{c} E_z \\ \frac{1}{c} E_x & & -B_z & B_y \\ \frac{1}{c} E_y & B_z & & -B_x \\ \frac{1}{c} E_z & -B_y & B_x & \end{pmatrix}$$

Geometrically, this is called a Tensor

We can check that the lorentz transformations are equivalent to

$$F' = L F L^T$$

$$\Leftrightarrow F'^{\mu\nu} = L^{\mu}_{\rho} F^{\rho\sigma} (L^T)_{\sigma}^{\nu}$$

$$\boxed{F'^{\mu\nu} = L^{\mu}_{\rho} L^{\nu}_{\sigma} F^{\rho\sigma}}$$

Note: Electromagnetism (Maxwell's equations) is already fully consistent with relativity, unlike Newtonian dynamics

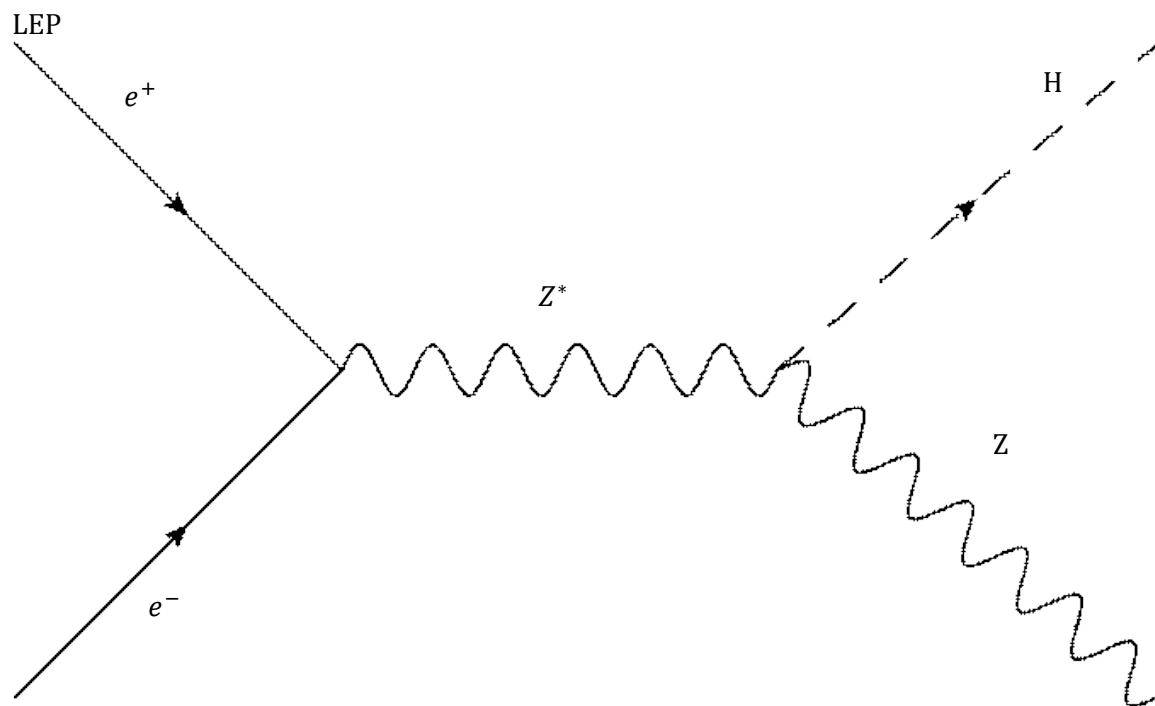
No EM in jan exam



# Higgs Boson

13 December 2011

10:28



$$E_{CM} = 206\text{GeV}$$
$$E_{beam} = 103\text{GeV}$$

Limit

$$m_H = 209 - 91$$
$$= 115\text{GeV}$$

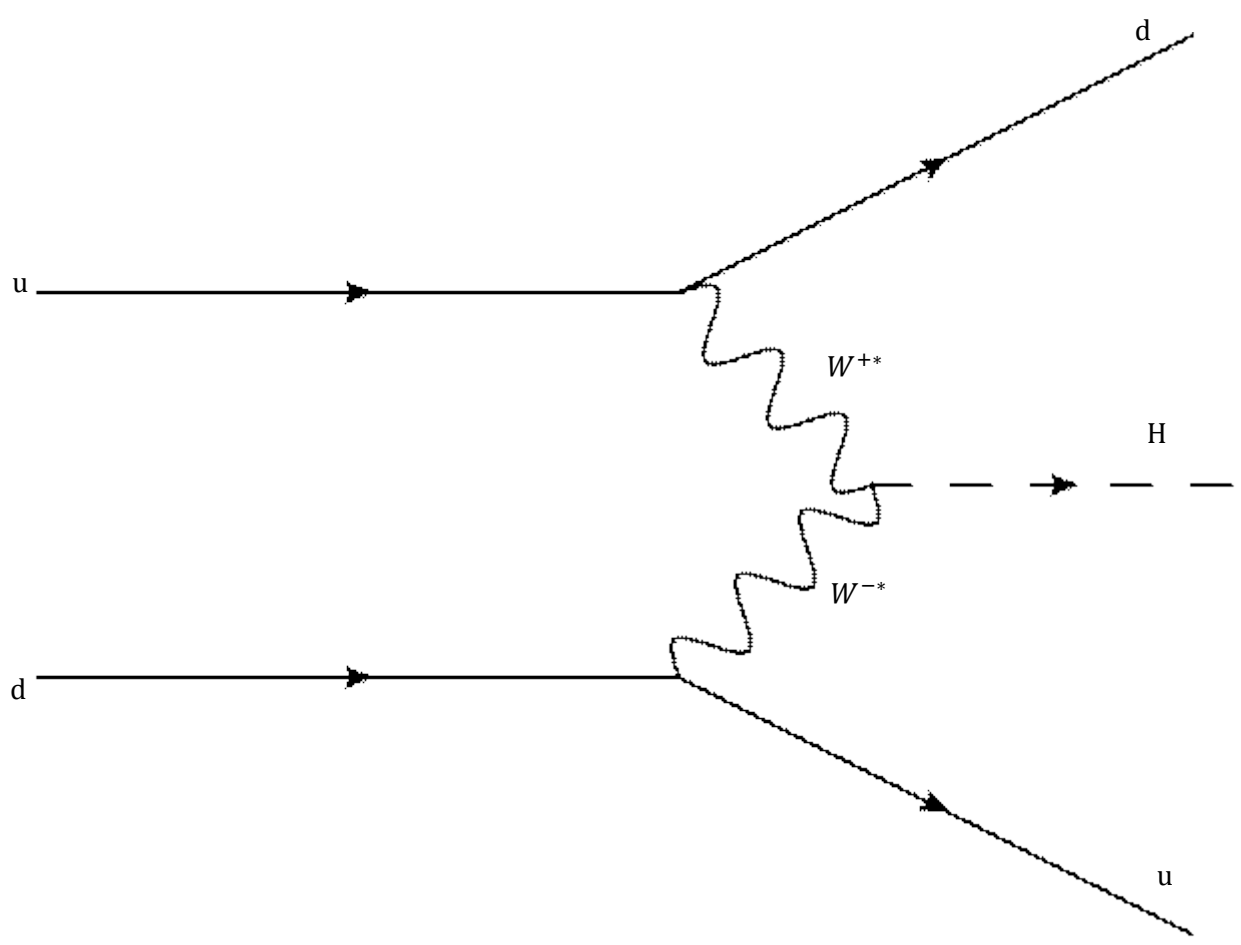
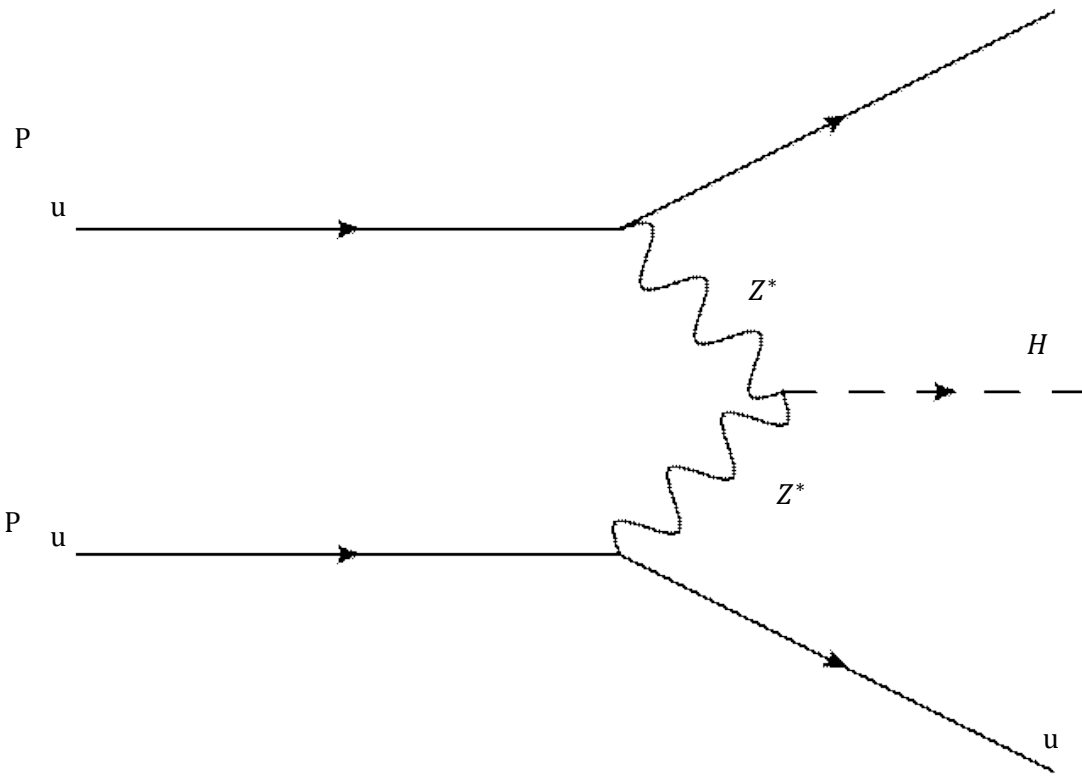
$$m_z = 91\text{GeV}$$

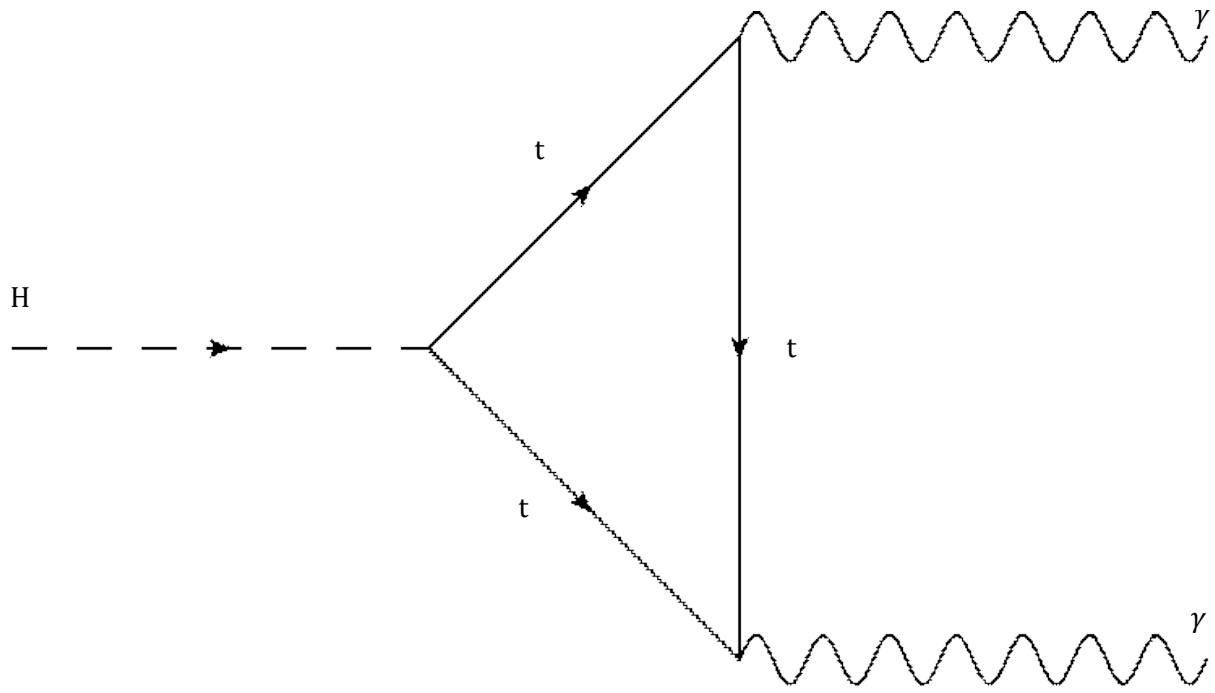
LEP didn't see H (shut down in 2000)

$$\Rightarrow m_H > 115\text{GeV}$$

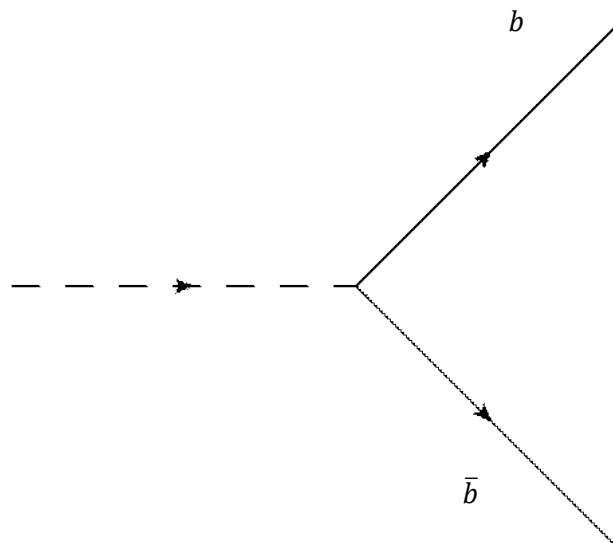
LHC

u





OR



$m_H \approx 126\text{GeV?}$

# Mathematical Methods

04 October 2011

10:55

Linear algebra  
Vector calculus

📖 Essential Mathematical Methods for the physical sciences

K.F. Riley and M. P. Hobson

CUP 2011

Cont assessment

4-5 exercise classes

~1 hour

MxN matrix: M rows and N columns

$$\text{Vector } \vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

Column vector

$$\vec{w} = (w_1 \quad w_2 \quad w_3)$$

Row vector

Transpose T

Swapping rows and columns

Trace of a matrix

$$\text{Tr } A = \sum \text{diagonal elements}$$

$$\sum_{i=1}^N a_{ii}$$

Multiplication

AB=C

$$c_{ij} = \sum_k a_{ik} b_{kj}$$

$AB \neq BA$

$$\text{Tr } C = \text{Tr } AB = \text{Tr } BA$$

$$\begin{aligned} \text{Tr } C &= \sum_i c_{ii} \\ &= \sum_i \sum_k a_{ik} b_{ki} \\ &= \sum_{ijk} b_{ki} a_{ik} \\ &= \text{tr } BA \end{aligned}$$

$$\text{Tr } BCA = \text{tr } CAB = \text{tr } BCA$$

Linear Algebra

Vectorspace  $\vec{v}$

$$\vec{w} + \vec{v} = \vec{u} \text{ addition}$$

$$\lambda \vec{v} = \vec{w} \text{ multiplication}$$

A+B=C provided that they are the same size

$$\lambda A = B \quad \lambda \in \mathbb{C}$$

$$(A + B)\vec{v} = A\vec{v} + B\vec{v}$$

$$A(\lambda \vec{v}) = \lambda A\vec{v}$$

Products AB,  $AA = A^2$

$A \dots A = A^n$   
 $n$   
 Functions of matrices  
 $e^A$

$$e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \dots = \sum_{n=0}^{\infty} \frac{1}{n!} x^n$$

$$e^A = \sum_{n=0}^{\infty} \frac{1}{n!} A^n$$

⇒ evaluate this bitches!

This is fundamental in QM

Heisenberg matrix mechanics

Hamiltonian H

Time evolution  $e^{iHt}$

□ Book: section 1.1-1.5

### Inverse

Numbers  $y = ax \quad x = \frac{1}{a}y = a^{-1}y$

$$\bar{y} = A\bar{x}$$

$$\bar{x} = A^{-1}\bar{y}$$

2x2 example  $y = Ax; \quad x = A^{-1}y$

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$\begin{cases} y_1 = ax_1 + bx_2 & .c \\ y_2 = cx_1 + dx_2 & .a \end{cases}$$

$$cy_1 - ay_2 = acx_1 + bcx_2 - acx_1 - adx_2 = (bc - ad)x_2$$

$$x_2 = \frac{1}{bc - ad}(cy_1 - ay_2)$$

$$x_1 = \frac{1}{bc - ad}(by_2 - dy_1)$$

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = A^{-1}y$$

$$A^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

Inverse exists except when

$$ad - bc = 0$$

$A^{-1}$  exists, provided  $\det A \neq 0$

Properties (general, verify for 2x2 matrices)

Product rule:

$$\det AB = \det A \det B$$

$A^{-1}A = I = \text{identity matrix} (\det I = 1)$

$$\det A^{-1}$$

$$\det A^{-1}A = \det I = 1$$

$$= \det A^{-1} \det A \Rightarrow \det A^{-1} = \frac{1}{\det A}$$

$\det \kappa A$  multiply every matrix element by  $\kappa$

$$= \kappa^N \det A$$

Minor:

$M_{ij} = \det(\text{matrix with } i\text{'th row and } j\text{'th column deleted})$

$$A = \begin{pmatrix} 2 & 3 & 1 \\ -4 & 8 & 0 \\ 10 & -1 & 5 \end{pmatrix}$$

$$M_{11} = \begin{vmatrix} 8 & 0 \\ -1 & 5 \end{vmatrix} = 40 - 0 = 40$$

$$M_{12} = \begin{vmatrix} -4 & 0 \\ 10 & 5 \end{vmatrix} = -20$$

$$M_{13} = \begin{vmatrix} 2 & 1 \\ -4 & 0 \end{vmatrix} = 0 - (-4) = 4$$

$$\text{Cofactor } C_{ij} = (-1)^{i+j} M_{ij}$$

$$(-1)^{i+j} = 1 \text{ if } i + j \text{ is even, } -1 \text{ if odd}$$

$$\det A = \sum_{\substack{\text{along row} \\ \text{or column}}} A_{ij} C_{ij}$$

Ex: Expand along first row

$$\begin{aligned} \det A &= 2C_{11} + 3C_{12} + 1C_{13} \\ &= 2(-1)^2 M_{11} + 3(-1)^2 M_{12} + 1(-1)^4 M_{13} \\ &= 2 \times 40 + 3(-20) + 1(-76) \\ &= 80 + 60 - 76 = 64 \end{aligned}$$

Expand along second row

$$\begin{aligned} \det A &= -4C_{21} + 8C_{22} + 0C_{23} \\ &= -4(-1)^3 M_{21} + 8(-1)^4 M_{22} \\ &= 4 \begin{vmatrix} 3 & 1 \\ -1 & 5 \end{vmatrix} + 8 \begin{vmatrix} 2 & 1 \\ 10 & 5 \end{vmatrix} \\ &= 4(15 + 1) + 8(10 - 10) = 64 \end{aligned}$$

4x4 matrix

Minors are dets of 3x3 matrices

For 3x3

$$\begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = A_{11}A_{22}A_{33} + A_{12}A_{23}A_{31} + A_{13}A_{21}A_{32} - A_{11}A_{23}A_{32} - A_{12}A_{21}A_{33} - A_{22}A_{13}A_{31}$$

Special matrices

$$\begin{pmatrix} A_{11} & & & \\ & A_{22} & & \emptyset \\ & & A_{33} & \\ & \emptyset & & \dots \\ & & & & A_{NN} \end{pmatrix}$$

Diagonal matrix  $\text{diag}(A_{11}, A_{22}, A_{33}, \dots, A_{NN})$

$$\det A = A_{11}A_{22}A_{33} \dots A_{NN}$$

$$A^{-1} = \begin{pmatrix} \frac{1}{A_{11}} & & & \\ & \frac{1}{A_{22}} & & \emptyset \\ & & \frac{1}{A_{33}} & \\ & \emptyset & & \dots \\ & & & & \frac{1}{A_{NN}} \end{pmatrix}$$

Upper | lower triangular

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ & A_{22} & A_{23} \\ & & A_{33} \end{pmatrix}$$

$$\det(\begin{matrix} \square & & \\ & \square & \\ & & \square \end{matrix}) = A_{11} \begin{vmatrix} A_{22} & A_{23} \\ & A_{33} \end{vmatrix} + 0 + 0 = A_{11}A_{22}A_{33}$$

Transpose  $A^T$

$$(A^T)_{ij} = A_{ji}$$

$$\det(A^T) = \det A$$

Complex conjugate \*

$$A_{ij}^*$$

$$\det(A^*) = (\det A)^*$$

Hermitian conjugate

$$A^{\dagger} = A \text{ dagger} = A^{T*}$$

Symmetric matrices  $A^T = A$

Antisymmetric:  $A^T = -A$

Hermitian  $A^{\dagger} = A$

Antihermitian  $A^{\dagger} = -A$

Orthogonal matrices

$$A^T A = 1$$

Real matrix elements

2 vectors (real)

$\bar{x}, \bar{y}$

Interproduct

$$\bar{y}^T \bar{x}$$

$$\bar{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \quad \bar{y} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

$$\bar{y}^T = (y_1 \quad y_2 \quad y_3)$$

$$\bar{y}^T \bar{x} = \bar{y} * \bar{x}$$

$$(y_1 \quad y_2 \quad y_3) \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$y_1 x_1 + y_2 x_2 + y_3 x_3$$

$$\bar{x} \rightarrow A\bar{x}$$

$$\bar{y} \rightarrow A\bar{y}$$

$$(AB)^T = B^T A^T$$

$$\bar{y}^T \bar{x} \rightarrow (A\bar{y})^T A\bar{x} = \bar{y}^T A^T A \bar{x} = \bar{y}^T \bar{x}$$

Orthogonal transformation preserves the interproduct rotations

$$\det(A^T A) = \det 1 = 1$$

$$= \det A^T \det A = (\det A)^2$$

$$\det A = \pm 1 \quad (+1 \Rightarrow \text{rotations})$$

Complex numbers

$$\bar{x} \Rightarrow U\bar{x} \text{ unitary}$$

$$\bar{y} \rightarrow U\bar{y}$$

Unitary matrix

$$U^{\dagger} U = 1$$

Preserve inner product

$$\bar{y}^T \bar{x} \rightarrow (U\bar{y})^T U\bar{x}$$

$$= \bar{y}^{\dagger} U^{\dagger} U \bar{x} = \bar{y}^{\dagger} \bar{x}$$

# Eigenvalues and Eigenvectors

11 October 2011

11:05

Ex

$$A = \begin{pmatrix} 1 & 2 \\ 4 & -1 \end{pmatrix}$$

Consider a vector

$$\bar{w} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

$$A\bar{w} = \begin{pmatrix} 1 & 2 \\ 4 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 5 \\ 2 \end{pmatrix}$$

Nothing special

Let's now take

$$\bar{v} = \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

$$A\bar{v} = \begin{pmatrix} 1 & 2 \\ 4 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -2 \end{pmatrix} = \begin{pmatrix} -3 \\ 6 \end{pmatrix} = -3 \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

$\bar{v}$  is an eigenvector of A

$$A\bar{v} = \lambda\bar{v}$$

A=matrix

$\lambda$ = number (complex or real)

$\bar{v}$ =eigenvector of A

$\lambda$  is called an eigenvalue

⇒ appear all over physics

- Vibrations
- Crystals
- QM

Solve  $A\bar{v} = \lambda\bar{v}$  find  $\lambda$

$$\Rightarrow (A - \lambda I)\bar{v} = 0$$

$$\text{Always } \bar{v} = \begin{pmatrix} 0 \\ 0 \\ \dots \\ 0 \end{pmatrix}$$

Trivial solution: not interesting

Nontrivial solution

To have a nontrivial solution, should not be able to invert  $(A - \lambda I)$

$$\rightarrow \det(A - \lambda I) = 0$$

⇒ polynomial eq in  $\lambda$

⇒ *characteristic equation*

$$N * N \text{ matrix: } \lambda^N + \lambda^{N-1} + \dots + \lambda + c = 0$$

$$\text{Coefficient of } \lambda^{N-1} = \text{Tr } A$$

Check: proof will follow

$$\text{Tr } A = \sum_{i=1}^N \lambda_i \text{ (sum)}$$

$$\det A = \prod_{i=1}^N \lambda_i \text{ (product)}$$

In general,  $\lambda \in \mathbb{C}$

$$A \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

$$\det \begin{pmatrix} a - \lambda & b \\ c & d - \lambda \end{pmatrix}$$

$$= (a - \lambda)(d - \lambda) - bc = \lambda^2 - \lambda(a + d) + ad - bc = 0$$

$$\lambda = \frac{a + d}{2} \pm \frac{1}{2} \sqrt{(a + d)^2 - 4ad + 4bc}$$



$$\lambda = \frac{(a+d)}{2} \pm \frac{1}{2} \sqrt{(a-d)^2 + 4bc}$$

Complex if

$$(a-d)^2 + 4bc < 0$$

If  $b=c$

$$\lambda = \frac{(a+d)}{2} \pm \frac{1}{2} \sqrt{(a-d)^2 + 4b^2} > 0$$

Real

Symmetric matrix has real eigenvalues

Ex

$$A = \begin{pmatrix} a & b \\ b & c \end{pmatrix} = A^T$$

Eigenvalues/eigenvectors

$$A\bar{v} = \lambda\bar{v}$$

1.  $\lambda$  eigenvalue

$$\det(A - \lambda I) = 0$$

2. Find eigenvectors

Eigenvectors are determined uniquely except for the overall normalization. (they can have different magnitudes, but same direction)

If  $\bar{v}$  is an eigenvector, then  $\bar{v}' = \kappa\bar{v}$  is also eigenvector ( $\kappa \in \mathbb{C}$ )

$$A\bar{v} = \lambda\bar{v}$$

$$A\bar{v}' = A(\kappa\bar{v}) = \kappa A\bar{v} = \kappa\lambda\bar{v} = \lambda(\kappa\bar{v}) = \lambda\bar{v}'$$

Diagonal matrix

$$A = \begin{pmatrix} 1 & 2 \\ 4 & -1 \end{pmatrix}, \lambda = 3: \bar{v}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \lambda = -3: \bar{v}_2 = \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

$$D = \begin{pmatrix} 3 & 0 \\ 0 & -3 \end{pmatrix}$$

-eigenvalues in diagonal

We can transform A into D via a transformation called diagonalization

Let's combine the eigenvectors in a matrix S

$$S = (\bar{v}_1 \quad \bar{v}_2)$$

$$AS = A(\bar{v}_1 \quad \bar{v}_2)$$

Statement:

Similarity transformation

$$S^{-1}AS$$

Diagonalizes A

$$S = \begin{pmatrix} 1 & 1 \\ 1 & -2 \end{pmatrix}$$

$$S^{-1} = \frac{1}{-3} \begin{pmatrix} -2 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 2 & 1 \\ 1 & -1 \end{pmatrix}$$

Verify  $S^{-1}S = I$

$$S^{-1}AS = \frac{1}{3} \begin{pmatrix} 2 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 4 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -2 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 2 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 3 & 3 \\ 3 & -6 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 9 & 0 \\ 0 & -9 \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ 0 & -3 \end{pmatrix} = D$$

$$\text{Tr } AB = \text{Tr } BA$$

$$\Rightarrow \text{tr}(S^{-1}AS) = \text{tr } D = \sum_{i=1}^N \lambda_i$$

$$\text{Tr}(ASS^{-1}) = \text{tr } A$$

$$\det(AB) = \det A \det B$$

$$\det(S^{-1}AS) = \det D = \prod_{i=1}^N \lambda_i$$

$$\det S^{-1} \det A \det S = \det(SS^{-1}) \det A = \det A$$

Ex

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$A^T = A$$

$$\begin{aligned} \text{Tr } A &= 0 \\ \det A &= 0 \\ \Pi \lambda &= 0 \Rightarrow \text{at least 1 eigenvalue should be 0} \\ \Sigma \lambda &= 0 \Rightarrow \lambda = 0, +a, -a \end{aligned}$$

$$\begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{vmatrix} = -\lambda^3 + 2\lambda = 0$$

Characteristic eq

$$-\lambda(\lambda^2 - 2) = 0$$

$$\lambda = \begin{matrix} 0 \\ \sqrt{2} \\ -\sqrt{2} \end{matrix}$$

Eigenvectors

1.  $\lambda = 0$

$$A\bar{v} = 0\bar{v}, v = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{matrix} y = 0 \\ x + z = 0 \\ y = 0 \end{matrix} \Rightarrow \bar{v}_1 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

2.  $\lambda = \sqrt{2}$

$$A\bar{v} = \sqrt{2}\bar{v}$$

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \sqrt{2} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\begin{cases} y = \sqrt{2}x & x + z = 2x \\ x + z = \sqrt{2}y & \Rightarrow x = z \\ y = \sqrt{2}z & y = \sqrt{2}x \end{cases}$$

$$\bar{v}_2 = \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$$

3.  $\lambda = -\sqrt{2}$

$$\bar{v}_3 = \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

$$\Rightarrow S, S^{-1} \quad S^{-1}AS = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & -\sqrt{2} \end{pmatrix}$$

Matrix A

Eigenvalues  $\lambda$

$$\det(A - \lambda I) = 0$$

Eigenvectors  $\bar{v}$

$$A\bar{v} = \lambda\bar{v}$$

$$S = \begin{pmatrix} \bar{v}_1 & \bar{v}_2 & \bar{v}_3 \end{pmatrix}$$

$$S^{-1}AS = D$$

$$D = \begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3 \end{pmatrix}$$

$$\text{Tr } A = \sum_i \lambda_i$$

$$\det A = \prod_i \lambda_i$$

$$(AB)^{dag} = B^{dag} A^{dag}$$

Hermetian matrix

$$H^{dag} = H$$

Suppose  $\bar{v}$  is an eigenvector

$$H\bar{v} = \lambda\bar{v}$$

$$(H\bar{v})^{dag} = (\lambda\bar{v})^{dag}$$

$$\bar{v}^{dag}H^{dag} = \lambda^*\bar{v}^{dag}$$

$$= \bar{v}^{dag}H$$

$$H\bar{v} = \lambda\bar{v}$$

$$\bar{v}^{dag}H = \lambda^*\bar{v}^{dag}$$

$$\bar{v}^{dag}H\bar{v}$$

3 inner product

$$1: 3 = \bar{v}^{dag}\lambda\bar{v} = \lambda\bar{v}^{dag}\bar{v}$$

$$2 = \lambda^*\bar{v}^{dag}\bar{v} \Rightarrow$$

$$\lambda\bar{v}^{dag}\bar{v} = \lambda^*\bar{v}^{dag}\bar{v}$$

$$\bar{v}^{dag}\bar{v} > 0 \quad \bar{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}, \quad \bar{v}^{dag}\bar{v} = |v_1|^2 + |v_2|^2 + |v_3|^2 > 0$$

$$\Rightarrow (\lambda - \lambda^*)\bar{v}^{dag}\bar{v} = 0$$

$$\Rightarrow \lambda = \lambda^*$$

Real eigenvalue

if  $H^{dag} = H$ , then  $\lambda^* = \lambda$

Lets consider  $\lambda_1, \lambda_2$

$$\lambda_1 \neq \lambda_2$$

$$3 \quad H\bar{v}_1 = \lambda_1\bar{v}_1$$

$$4 \quad H\bar{v}_2 = \lambda_2\bar{v}_2$$

$$\bar{v}_2^{dag}H\bar{v}_1 = \bar{v}_2^{dag}\lambda_1\bar{v}_1 = \lambda_1\bar{v}_2^{dag}\bar{v}_1$$

$$= \lambda_2\bar{v}_2^{dag}\bar{v}_1$$

$$(\lambda_1 - \lambda_2)\bar{v}_2^{dag}\bar{v}_1 = 0$$

$$\Rightarrow \bar{v}_2^{dag}\bar{v}_1 = 0$$

Eigenvectors are orthogonal innerproduct = 0

Eigenvectors of hermitian matrix with distinct eigenvalues are orthogonal

Normalize eigenvectors

$$\text{If } \bar{v}_1^{dag}\bar{v}_1 = c$$

$$\text{Then } \bar{w}_1 = \frac{1}{\sqrt{c}}$$

is also an eigenvector

$$\text{And } \bar{w}_1^{dag}\bar{w}_1 = \frac{1}{\sqrt{c}}\frac{1}{\sqrt{c}}\bar{v}_1^{dag}\bar{v}_1 = 1 \text{ is normalized}$$

So

$$\bar{v}_1^{dag}\bar{v}_1 + \bar{v}_2^{dag}\bar{v}_2 = \bar{v}_2^{dag}\bar{v}_2 = 1$$

$$\bar{v}_1^{dag}\bar{v}_2 = 0$$

$\bar{v}_1$  and  $\bar{v}_2$  form an orthonormal set or a basis

$$\bar{v}_i^{dag}\bar{v}_j = \delta_{ij}$$

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

Hermitian matrix can be diagonalized by a unitary transformation

In general

$$S^{-1}AD = D$$

$$S^{-1}HS = D$$

$$D = \begin{pmatrix} \lambda_1 & & \\ & \dots & \\ & & \lambda_N \end{pmatrix} = D^{dag}$$

So

$$D^{dag} = D = (S^{-1}HS)^{dag} = S^{dag}H^{dag}S^{-1dag} = S^{dag}HS^{-1dag}$$

$$\Rightarrow S^{-1}HS = S^{dag}HS^{-1dag}$$

$$S^{dag} = S^{-1} \Rightarrow S \text{ is unitary}$$

$$U^{dag}HU = D$$

All of this holds also for symmetric real matrices

$$A, A_{ij} \in \mathbb{R}$$

$$A^T = A$$

$$\lambda \in \mathbb{R}$$

$$\bar{v}_i^T \bar{v}_j = \delta_{ij}$$

$$O^T A O = D$$

Orthogonal transformation

Ex

$$H = \begin{pmatrix} 2 & 2-i \\ 2+i & 6 \end{pmatrix} = H^{dag}$$

$$\text{Tr}H = 2 + 6 = 8$$

$$\det H = 2 * 6 - (2+i)(2-i) = 12 - 4 - 1 = 7$$

Eigenvalues

$$\det(H - \lambda I) = \begin{vmatrix} 2-\lambda & 2-i \\ 2+i & 6-\lambda \end{vmatrix} = (2-\lambda)(6-\lambda) - (2+i)(2-i)$$

$$\lambda^2 - 8\lambda + 7 = (\lambda - 7)(\lambda - 1) = 0$$

$$\lambda_1 = 7, \lambda_2 = 1$$

$$\lambda_i: H\bar{v}_1 = 7\bar{v}_1 \Rightarrow \begin{pmatrix} 2 & 2-i \\ 2+i & 6 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 7 \begin{pmatrix} x \\ y \end{pmatrix}$$

$$2 + (2-i)y = 7x: 5x = (2-i)y$$

$$(2+i)x + 6y = 7y: y = (2+i)x$$

$\Rightarrow$  solution

$$\begin{matrix} x = 1 \\ y = 2+i \end{matrix} \Rightarrow \bar{v}_1 = \begin{pmatrix} 1 \\ 2+i \end{pmatrix}, \bar{v}_1^{dag} \bar{v}_1 = (1 \quad 2-i) \begin{pmatrix} 1 \\ 2-i \end{pmatrix} = 1 + 5 = 6$$

Normalize

$$\bar{v}_1 = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 2+i \end{pmatrix}, H\bar{v}_1 = 7\bar{v}_1, \bar{v}_1^{dag} \bar{v}_1 = 1$$

$$\lambda_2 = 1: H\bar{v}_2 = 1\bar{v}_2$$

$$\begin{pmatrix} 2 & 2-i \\ 2+i & 6 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix}$$

$$2x + (2-i)y = x \Rightarrow x = -(2-i)y \Rightarrow x = -2 + i$$

$$(2+i)x + 6y = y \Rightarrow 5y = -(2+i)x \Rightarrow y = 1$$

$$\bar{v}_2 = \begin{pmatrix} -2+i \\ 1 \end{pmatrix}$$

$$\bar{v}_2^{dag} \bar{v}_2 = 1 + 5 = 6$$

$$\Rightarrow \bar{v}_2 = \frac{1}{\sqrt{6}} \begin{pmatrix} -2+i \\ 1 \end{pmatrix}$$

test

$$\bar{v}_2^{dag} \bar{v}_1 = 0?$$

$$\frac{1}{\sqrt{6}} \frac{1}{\sqrt{6}} (-2-i \quad 1) \begin{pmatrix} -2+i \\ 1 \end{pmatrix} = \frac{1}{6} (-2-i+2+i) = 0$$

$$U = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{-2+i}{\sqrt{6}} \\ \frac{2+i}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & -2+i \\ -2-i & 1 \end{pmatrix}$$

$$U^{dag} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 2-i \\ -2-i & 1 \end{pmatrix}$$

$$U^{dag}U = \frac{1}{(\sqrt{6})^2} \begin{pmatrix} 1 & 2-i \\ -2-i & 1 \end{pmatrix} \begin{pmatrix} 1 & -2+i \\ -2-i & 1 \end{pmatrix} = \frac{1}{6} \begin{pmatrix} 1+5 & 0 \\ 0 & 1+5 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$U^{dag}HU = \dots = \begin{pmatrix} 7 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\begin{array}{l} A = S^{-1}AS = D \\ H^{dag} = H:U^{dag}HU = D \\ A^T = A:O^{dag}AO = D \end{array}$$

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!} = \frac{1}{0!} + \frac{A}{1!} + \frac{A^2}{2!} + \frac{A^3}{3!} + \dots$$

$$A^n = SDS^{-1}SDS^{-1}SDS^{-1} \dots SDS^{-1} = SD^nS^{-1}$$

$$\Rightarrow \boxed{A = SDS^{-1}}$$

$$D = \begin{pmatrix} f_1 & & \emptyset \\ & f_2 & \\ \emptyset & & \dots \\ & & & f_n \end{pmatrix}, D^2 = \begin{pmatrix} f_1^2 & & \emptyset \\ & f_2^2 & \\ \emptyset & & \dots \\ & & & f_n^2 \end{pmatrix}, D^n = \begin{pmatrix} f_1^n & & \emptyset \\ & f_2^n & \\ \emptyset & & \dots \\ & & & f_n^n \end{pmatrix}$$

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!} = \sum_{n=0}^{\infty} S \frac{D^n}{n!} S^{-1} = S \left( \sum_{n=0}^{\infty} \frac{D^n}{n!} \right) S^{-1}$$

$$\sum_{n=0}^{\infty} \frac{D^n}{n!} = \begin{pmatrix} \sum_{n=0}^{\infty} \frac{f_1^n}{n!} & & \emptyset \\ & \sum_{n=0}^{\infty} \frac{f_2^n}{n!} & \\ \emptyset & & \dots \\ & & & \sum_{n=0}^{\infty} \frac{f_n^n}{n!} \end{pmatrix}$$

It's because we don't have  $D^n$  but  $\sum D^n$  you also sum each matrix to get this result

$$= \begin{pmatrix} e^{f_1} & & \emptyset \\ & e^{f_2} & \\ \emptyset & & \dots \\ & & & e^{f_n} \end{pmatrix}$$

$$e^A = Se^D S^{-1}$$

$$\det A = \det(Se^D S^{-1}) = \det S \det e^D \det S^{-1} = \det e^D$$

$$\begin{pmatrix} e^{\lambda_1} & & \emptyset \\ & e^{\lambda_2} & \\ \emptyset & & \dots \\ & & & e^{\lambda_N} \end{pmatrix} = e^D$$

$$e^A = Se^D S^{-1}$$

$$\det e^A = \det Se^D S^{-1} = \det S \det e^D \det S^{-1} = \det e^D$$

$$\det A = \prod_i \lambda_i$$

$$\det e^D = e^{\lambda_1} e^{\lambda_2} e^{\lambda_3} \dots e^{\lambda_N} = e^{\lambda_1 + \lambda_2 + \lambda_3 + \dots + \lambda_N} = e^{\sum_i \lambda_i} = e^{\text{Tr}(A)}$$

$$\det e^D = e^{\text{Tr}(A)}$$

Expand

$$e^A e^B = \left( 1 + A + \frac{A^2}{2} + \dots \right) \left( 1 + B + \frac{B^2}{2} + \dots \right) = 1 + A + B + \frac{A^2}{2} + \frac{B^2}{2} + AB + \dots$$

$$e^{A+B} = 1 + A + B + \frac{1}{2}(A+B)(A+B) + \dots$$

$$= 1 + A + B + \frac{1}{2}(A^2 + AB + BA + B^2) + \dots$$

They differ!

$$AB \leftrightarrow \frac{1}{2}(AB + BA)$$

$$AB \neq BA!$$

$$e^A e^B \neq e^{A+B}$$

$$[A, B] = AB - BA$$

Correct for the mismatch by adding commutators

$$\frac{1}{2}(AB + BA) + \frac{1}{2}[A, B] = AB$$

Campbell-baker-hausdorff formula

$$e^A e^B = e^{A+B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] - \frac{1}{2}[B, [A, B]] + \dots}$$

$$[B, [A, B]] * B[A, B] - [A, B]B = B(AB - BA) - (AB - BA)B$$

Suppose we have two hermitian N\*N matrices

$$A = A^{dag}, B = B^{dag}$$

When do these have a common set of eigenvectors?

Can be diagonalized simultaneously?

Answer: if A and B commute

$$[A, B] = AB - BA = 0$$

i)  $A\bar{v}_i = \lambda_i \bar{v}_i, \lambda_i$  all different

Lets assume  $AB=BA$

$$AB\bar{v}_i = BA\bar{v}_i = B\lambda_i \bar{v}_i = \lambda_i B\bar{v}_i$$

$$\Rightarrow A(B\bar{v}_i) = \lambda(B\bar{v}_i)$$

If  $\bar{v}_i$  is the eigenvector of A, then so is  $B\bar{v}_i$  with the same eigenvalue

Every eigenvector is uniquely determined up to normalization

$$B\bar{v}_i \sim \bar{v}_i$$

$$\Rightarrow B\bar{v}_i = \mu_i \bar{v}_i, \mu_i \text{ scalar}$$

$\bar{v}_i$  is indeed an eigenvector of B with eigenvalues  $\mu_i$

ii) Let's assume

$$A\bar{v}_i = \lambda_i \bar{v}_i$$

$$B\bar{v}_i = \mu_i \bar{v}_i$$

Common set of eigenvectors

$$\bar{v}_i + \bar{v}_i = \delta_{ij}$$

Orthogonal set basis

Every vector can be written as

$$\bar{x} = \sum_i c_i \bar{v}_i$$

$$AB\bar{x} = \sum_i c_i \lambda_i \mu_i \bar{v}_i$$

$$BA\bar{x} = \sum_i c_i \lambda_i \mu_i \bar{v}_i$$

$$\Rightarrow AB\bar{x} = BA\bar{x} \forall \bar{x}$$

$$AB = BA$$

Commute!

### Degenerate eigenvalues

If  $H = H^{dag}$  or  $M^T = M$  then eigenvectors form a basis, i.e. they form an orthogonal set

$$\bar{v}_i^{dag} \bar{v}_j = \delta_{ij}$$

$i, j$  label the eigenvectors

$$= 1 \text{ if } i = j$$

$$\delta_{ij} = 0 \text{ if } i \neq j$$

This is true when all  $\lambda_i$ 's are distinct. If some  $\lambda_i$ 's are degenerate (equal), this is correct, but requires still some more work

$$A = \begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix}$$

$$A^T = A; \lambda \in \mathbb{R}$$

$$Tr A = 0$$

$$\det A = -2 + 0 + 0 - 0 - 0 + 18 = 16$$

$$\det(A - \lambda \mathbb{I}) = \begin{vmatrix} 1-\lambda & 0 & 3 \\ 0 & -2-\lambda & 0 \\ 3 & 0 & 1-\lambda \end{vmatrix} = (-2-\lambda) \begin{vmatrix} 1-\lambda & 3 \\ 3 & 1-\lambda \end{vmatrix} = -(\lambda+2)((\lambda-1)^2 - 9)$$

$$= 0$$

$$\lambda = -2$$

$$(\lambda - 1)^2 - 9 = 0 \Rightarrow (\lambda - 1)^2 = 9$$

$$\lambda - 1 = \pm 3: \lambda = 4, \quad \lambda = -2$$

$$\lambda = 4, -2, -2$$

Degenerate

$$\lambda = 4: \begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 4 \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\begin{aligned} x + 3z &= 4x & x &= z \\ -2y &= 4y & \Rightarrow y &= 0 \\ 3x + z &= 4z & x &= z \end{aligned} \Rightarrow \bar{v} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \bar{v}^{dag} \bar{v} = 1$$

$$\lambda = -2: \begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = -2 \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\begin{aligned} x + 3z &= -2x & x &= -z \\ -2y &= -2y & \Rightarrow y &= y \\ 3x + z &= -2z & x &= -z \end{aligned} \Rightarrow \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix}, \begin{pmatrix} a \\ b \\ -a \end{pmatrix}$$

All eigenvectors

Chose two eigenvectors and make them orthogonal

$$\Rightarrow \bar{v}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \bar{v}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Now

$$\bar{v}_i^{dag} \bar{v}_j = \delta_{ij}$$

$$\bar{v}_3 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} \text{ is eigenvector}$$

But not orthogonal to  $\bar{v}_2$

★ BB: sheet with algebra

# Vector calculus and Integration

01 November 2011

14:46

2d 3d integrals-> integral theorem

Conservative vector fields => em maxwell equations

$$\int_a^b f(x) dx$$

Divide interval  $a < x < b$  in  $N$  subintervals of length  $\Delta x$  such that  $b - a = N\Delta x$

In each interval pick a point  $x_i$ ;  $i=1, \dots, N$

Assume  $f(x)$  is constant in each subinterval

Add together the area for each subinterval

$$\sum_{i=1}^N \Delta x f(x_i)$$

This becomes a better approximation as  $\Delta x \rightarrow 0$

Definition

$$\int_a^b f(x) dx = \lim_{N \rightarrow \infty} \sum_{i=1}^N \Delta x f(x_i)$$

With

$$N\Delta x = b - a \Rightarrow \Delta x \rightarrow 0 \text{ if } \frac{b-a}{N}, N \rightarrow \infty$$

$$\boxed{\int_a^b f(x) dx = \lim_{N \rightarrow \infty} \sum_{i=0}^N f(x_i) \Delta x}$$

$$\iint dx dy xy = \int_0^1 \int_0^{\sqrt{1-x^2}} xy = \frac{1}{8}$$

for  $x^2 + y^2 = 1$

$$r = \sqrt{x^2 + y^2}$$

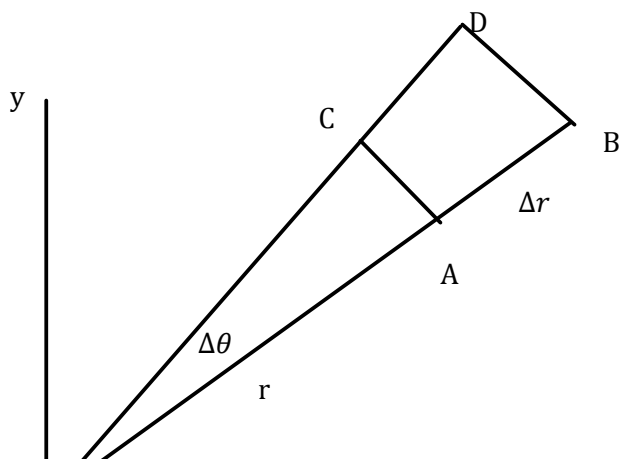
$$x = r \cos \theta$$

$$y = r \sin \theta$$

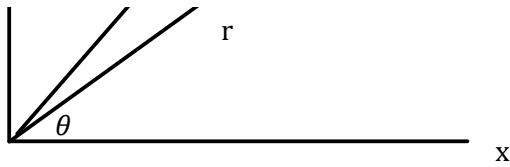
$$0 < r < 1$$

$$0 < \theta < \frac{\pi}{2}$$

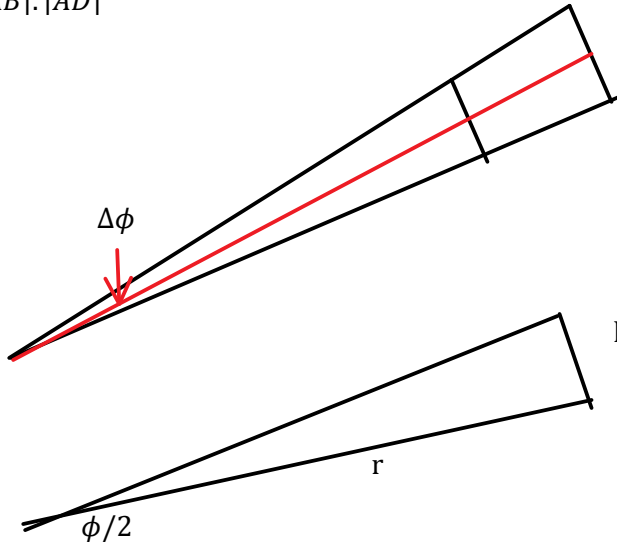
$$\iint dx dy f(x, t) \Rightarrow \int_0^1 dr \int_0^{\frac{\pi}{2}} d\theta \dots$$







$$|AB| \cdot |AD|$$



$$|AB| = \Delta r$$

$$|AD| = ?$$

$$l = r \sin\left(\frac{\Delta\phi}{2}\right)$$

$$|AD| = 2l = 2r \sin\left(\frac{\Delta\phi}{2}\right)$$

$$\Delta\phi \rightarrow 0$$

$$|AD| \rightarrow 2r \frac{\Delta\phi}{2} = r\Delta\phi$$

$$\phi \rightarrow \theta$$

$$|AB||AD| = \Delta r r \Delta\phi$$

$$= r \Delta r \Delta\theta$$

Jacobian:

$$J = r$$

For polar coordinates

$$\iint dx dy f(x, t) = \iint dr d\theta r f(r \cos \theta, r \sin \theta)$$

$$\iint dx dy 1 = \text{area}$$

$$\int_0^a dr \int_0^{2\pi} d\theta r 1 = \int_0^a dr r \int_0^{2\pi} d\theta = \frac{1}{2} r^2 \Big|_0^a \theta \Big|_0^{2\pi} = \frac{a^2}{2} 2\pi = \pi a^2$$

$$\iint dx dy xy$$

$$- \int_0^1 dr \int_0^{\frac{\pi}{2}} d\theta r r \cos \theta r \sin \theta$$

$$\int_0^1 dr r^3 \int_0^{\frac{\pi}{2}} d\theta \cos \theta \sin \theta = \left(\frac{1}{4} r^4 \Big|_0^1\right) \left(-\frac{1}{2} \cos^2 \theta \Big|_0^{\frac{\pi}{2}}\right) = \frac{1}{4} * \left(-\frac{1}{2}(0 - 1)\right) = \frac{1}{8}$$

$$\frac{d}{d\theta}(\cos^2 \theta) = 2 \cos \theta \frac{d \cos \theta}{d\theta} = -2 \cos \theta \sin \theta$$

$$\frac{d}{d\theta}(\sin^2 \theta) = 2 \sin \theta \frac{d \sin \theta}{d\theta} = 2 \sin \theta \cos \theta$$

$$\iint dx dy \sqrt{x^2 + y^2}$$

From 1 to 2

$$\int_1^2 dr \int_0^\pi d\theta r r = \int_1^2 dr r^2 \int_0^\pi d\theta = \frac{1}{3} r^3 \Big|_1^2 \pi = \frac{\pi}{3} (8 - 1) = \frac{7\pi}{3}$$

### 3d integrals

$$\int \int \int dx dy dz f(x, y, z)$$

Ex

$$f = 1$$

$$\int \int \int dx dy dz 1 = \text{volume of } v$$

Ex

$$f(x, y, z) = n(x, y, z)$$

Mass density  $\left[\frac{\text{kg}}{\text{m}^3}\right]$

$$\int \int \int_v dx dy dz n(x, y, z) = M = \text{total mass inside volume}$$

$$\int_0^a dx \int_0^a dy \int_0^a dz 1$$

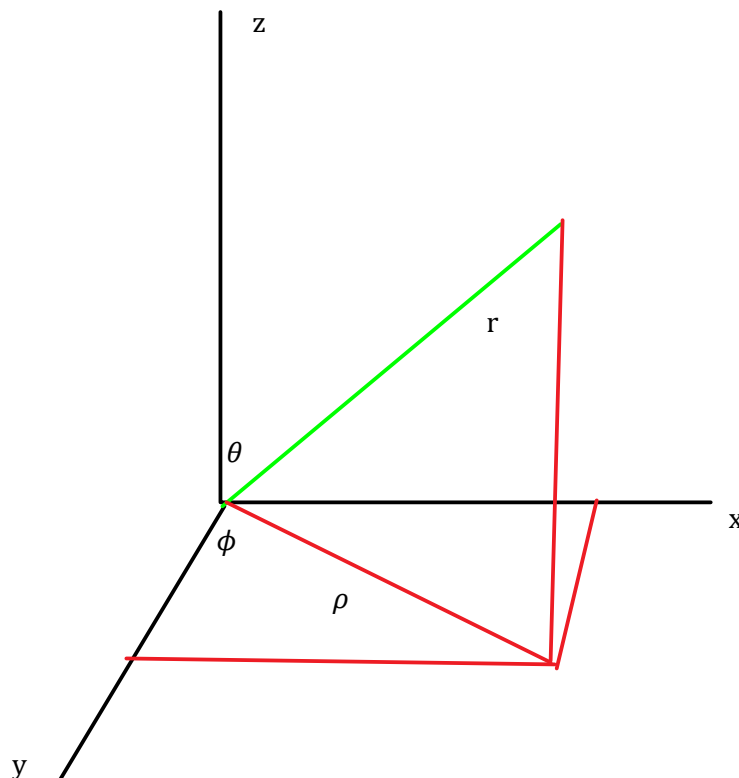
$$= x \Big|_0^a y \Big|_0^a z \Big|_0^a = a * a * a = a^3$$

Sphere radius a volume

$$\frac{4}{3} \pi a^3$$

Rotational symmetry

⇒ spherical coordinates



Last time: 2d, 3d integral

Rotational symmetry

2D:

Polar coordinates

$$x = r \cos \phi$$

$$y = r \sin \phi$$

$$r = \sqrt{x^2 + y^2}$$

$$\iint dx dy f(x, y)$$

$$= \int dr \int d\phi r f(r \cos \phi, r \sin \phi)$$

Inc jacobian r

$$-\infty < x, y < \infty$$

$$0 < r < \infty$$

$$0 < \phi < 2\pi$$

$$y > 0 \leftrightarrow 0 < \phi < \pi$$

3D

$$\bar{r} = (x, y, z)$$

$$r, \phi, \theta$$

$\rho$  = projection in xy-plane

$$\rho = r \sin \theta$$

$$x = r \cos \phi \sin \theta$$

$$y = r \sin \phi \sin \theta$$

$$z = r \cos \theta$$

Spherical coordinates

$$-\infty < x, y, z < \infty$$

$$0 < r < \infty$$

$$0 < \phi < 2\pi$$

$$0 < \theta < \pi$$

$$\iiint dx dy dz f(x, y, z)$$

$$\int dr \int d\phi \int d\theta J f(x, y, z)$$

J=jacobian "change of variables"

Jacobian for spherical coordinates

$$J = r^2 \sin \theta$$

Ex

Sphere

$$0 < r < a$$

$$0 < \phi < 2\pi$$

$$0 < \theta < \pi$$

Volume of this sphere

$$\int_0^a dr \int_0^{2\pi} d\phi \int_0^\pi d\theta r^2 \sin \theta$$

$$\int_0^a dr r^2 \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta$$

$$\left[ \frac{1}{3} r^3 \right]_0^a \left[ \phi \right]_0^{2\pi} \left[ -\cos \theta \right]_0^\pi$$

$$= \frac{a^3}{3} * 2\pi * (-(-1) - (-1))$$

$$= \frac{4\pi}{3} a^3$$

Hemisphere

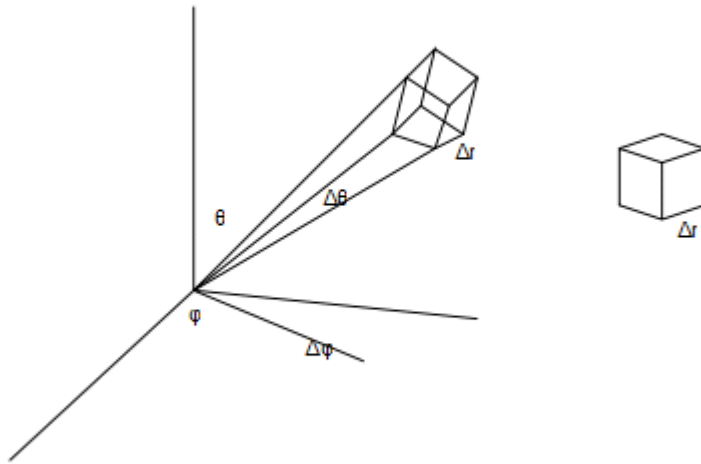
$$0 < \theta < \frac{\pi}{2}$$

Jacobian is the elementary volume, obtained by changing

$$r \rightarrow r + \Delta r$$

$$\theta \rightarrow \theta + \Delta \theta$$

$$\phi \rightarrow \phi + \Delta \phi$$



[ in cartesian coordinates ]  
 $\Delta x \Delta y \Delta z$

$r \rightarrow r + \Delta r$   
 One side  $\Delta r$

$\theta \rightarrow \theta + \Delta \theta$   
 $2r \sin\left(\frac{\Delta \theta}{2}\right)$   
 $\rightarrow r \Delta \theta$

$\Delta r \ r \Delta \theta \ r \sin \theta \ \Delta \phi$   
 $= r^2 \sin \theta \ \Delta r \ \Delta \theta \Delta \phi$   
 $r^2 \sin \theta = \text{jacobian}$

# Partial differentiation

16 November 2011

11:04

1 variable  $x$ ,  $f(x)$

2 variables  $f(x,t)$

Partial derivatives

$$\frac{\delta f(x, y)}{\delta x}, y \text{ is fixed}$$

$$\frac{\delta f(x, y)}{\delta y}, x \text{ is fixed}$$

3 2nd derivatives

$$\frac{\delta^2 f}{\delta x^2}, \frac{\delta^2 f}{\delta y^2}, \frac{\delta^2 f}{\delta x \delta y} = \frac{\delta^2 f}{\delta y \delta x}$$

Ex  $f(x, y) = x^3 y + y^2 \sin x$

$$\frac{\delta f}{\delta x} = 3x^2 y + y^2 \cos x$$

$$\frac{\delta f}{\delta y} = x^3 + 2y \sin x$$

$$\frac{\delta^2 f}{\delta x^2} = 6xy - y^2 \sin x$$

$$\frac{\delta^2 f}{\delta y^2} = 2 \sin x$$

$$\frac{\delta}{\delta y} \left( \frac{\delta f}{\delta x} \right) = \frac{\delta}{\delta x} \left( \frac{\delta f}{\delta y} \right) = 3x^2 + 2y \cos x = \frac{\delta^2 f}{\delta x \delta y}$$

Change of variables

1D

$$\int dy f(x)$$

$$x=x(u)$$

$$dx = \left( \frac{\delta x}{\delta u} \right) du$$

$$\int du \left( \frac{\delta x}{\delta u} \right) f(x(u))$$

$$\frac{\delta x}{\delta u} \rightarrow \text{jacobian}$$

Ex

$$\int_0^{\sqrt{\pi}} dx x \sin x^2$$

$$x = \sqrt{u}$$

$$dx = \frac{\delta x}{\delta u} du = \frac{1}{2\sqrt{u}} du$$

$$= \int_0^{\pi} du \frac{1}{2\sqrt{u}} \sqrt{u} \sin u$$

$$= \int_0^{\pi} du \frac{1}{2} \sin u$$

$$= -\frac{1}{2} \cos u \Big|_0^{\pi} = 1$$

Change of variables in more dimensions

$(x,y,z) \rightarrow (u,v,w)$

Ie

$$x=x(u,v,w)$$

$$y=y(u,v,w)$$

$$z = z(u, v, w)$$

Here

$$\frac{\delta x}{\delta u}, \frac{\delta x}{\delta v}$$

$$\frac{\delta y}{\delta u}$$

Ex

9 different partial derivatives

Jacobian = absolute value of

$$\det \begin{pmatrix} \frac{\delta x}{\delta u} & \frac{\delta x}{\delta v} & \frac{\delta x}{\delta w} \\ \frac{\delta y}{\delta u} & \frac{\delta y}{\delta v} & \frac{\delta y}{\delta w} \\ \frac{\delta z}{\delta u} & \frac{\delta z}{\delta v} & \frac{\delta z}{\delta w} \end{pmatrix} = \frac{\delta(x, y, z)}{\delta(u, v, w)}$$

$$\iiint dx dy dz f(x, y, z) = \iiint du dv dw \left| \frac{\delta(x, y, z)}{\delta(u, v, w)} \right| f(x(u, v, w), y(\square), z(\square))$$

Ex 2d polar coordinates

$$x = x(r, \phi) = r \cos \phi$$

$$y = y(r, \phi) = r \sin \phi$$

$$\frac{\delta(x, y)}{\delta(r, \phi)} = \det \begin{pmatrix} \frac{\delta x}{\delta r} & \frac{\delta x}{\delta \phi} \\ \frac{\delta y}{\delta r} & \frac{\delta y}{\delta \phi} \end{pmatrix} = \det \begin{pmatrix} \cos \phi & -r \sin \phi \\ \sin \phi & r \cos \phi \end{pmatrix} = r \cos^2 \phi + r \sin^2 \phi = r$$

Ex 3d Spherical coordinates

$$(x, y, z) \rightarrow (r, \phi, \theta)$$

$$x = r \cos \phi \sin \theta$$

$$y = r \sin \phi \sin \theta$$

$$z = r \cos \theta$$

$$c\phi = \cos \phi$$

$$s\theta = \sin \theta$$

$$\frac{\delta(x, y, z)}{\delta(r, \phi, \theta)} = \det \begin{pmatrix} c\phi s\theta & -rs\phi s\theta & rc\phi c\theta \\ s\phi s\theta & rc\phi s\theta & rs\phi c\theta \\ c\theta & 0 & -rs\theta \end{pmatrix} = \pm r^2 \sin \theta$$

$$J = \left| \frac{\delta(x, y, z)}{\delta(r, \phi, \theta)} \right| = r^2 \sin \theta$$

Ex  $\int_p dx dy xy$

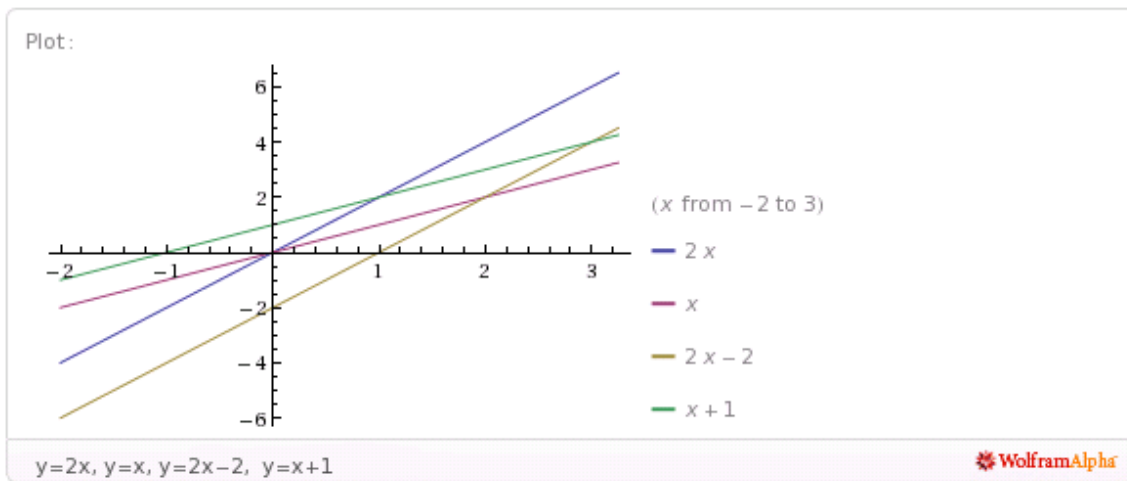
p = bounded region

$$y = 2x,$$

$$y = x,$$

$$y = 2x - 2,$$

$$y = x + 1$$



### Change of variables

$$x = u - v$$

$$y = 2u - v$$

$$\det \begin{pmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} \end{pmatrix} = \begin{vmatrix} 1 & -1 \\ 2 & -1 \end{vmatrix} = -1 + 2 = 1$$

$$\iint du dv 1(u - v)(2u - v)$$

Boundaries

$$y = 2x: 2u - v = 2(u - v): v = 0$$

$$y = 2x - 2: 2u - v = 2u - 2v - 2: v = -2$$

$$y = x: 2u - v = u - v: u = 0$$

$$y = x + 1: 2u - v = u - v + 1: u = 1$$

$$-2 < v < 0$$

$$0 < u < 1$$

$$\int_{-2}^0 dv \int_0^1 du (u - v)(2u - v)$$

$$= \int_{-2}^0 dv \int_0^1 du (2u^2 - 3uv + v^2) = 7$$

# Line integrals

16 November 2011

11:38

Work done by force

Particle  $m\vec{a} = \vec{F}$

3d:  $\vec{F}(\vec{r}) = (F_x(\vec{r}), F_y(\vec{r}), F_z(\vec{r}))$

Vector field

*Work = distance \* force*

Ex simplest

Particle moves in straight line

Constant force

$$\vec{F} = (F_x, F_y, F_z)$$

Displacement

$$\vec{r}_2 - \vec{r}_1$$

Work:

$$\vec{F} \cdot (\vec{r}_2 - \vec{r}_1)$$

$$= F_x(x_2 - x_1) + F_y(y_2 - y_1) + F_z(z_2 - z_1)$$

Curved path

Nonconstant force

Consider a small interval

$$\vec{r} \rightarrow \vec{r} + \Delta\vec{r}$$

$\vec{F}(\vec{r})$  is approximately constant

$$W_{\Delta\vec{r}} \approx \vec{F}(\vec{r}) \cdot \Delta\vec{r}$$

Add all small contributions together

Total work

$$W = \sum_{i=1}^N F(\vec{r}_i) \Delta\vec{r}_i$$

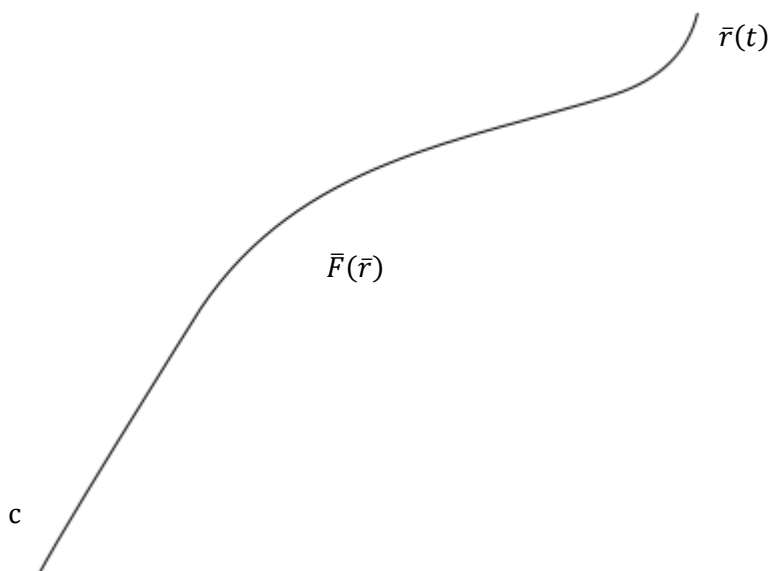
$$N \rightarrow \infty$$

$$W = \int_c \vec{F}(\vec{r}) d\vec{r}$$

Line integral

Work:

$$\int_c \vec{F}(\vec{r}) d\vec{r} = W$$





c /

Mechanics

$\vec{r}(t)$

t=time

$\vec{F}(\vec{r})$

$$\vec{F} = m\vec{a} = m \frac{d^2\vec{r}}{dt^2}$$

$$\vec{a} = \frac{d\vec{v}}{dt}$$

$$\vec{v} = \frac{d\vec{r}}{dt}$$

$$w = \int \vec{F} d\vec{r}$$

$$= m \int \frac{d^2\vec{r}}{dt^2} d\vec{r}$$

$\vec{r}(t) \rightarrow t$

Jacobian:

$$d\vec{r}(t) = \frac{d\vec{r}}{dt} dt$$

$$W = m \int dt \frac{d\vec{r}}{dt} * \frac{d^2\vec{r}}{dt^2} = m \int dt \vec{v} \frac{d}{dt} \vec{v}$$

$$\vec{v} \frac{d}{dt} \vec{v} = \frac{1}{2} \frac{d}{dt} (\vec{v}^2)$$

$$= m \int dt \frac{d}{dt} \left( \frac{1}{2} \vec{v}^2 \right) = \frac{1}{2} m \vec{v}^2 \Big|_{t_{initial}}^{t_{final}} = \Delta \text{kinetic energy} = \text{work}$$

$$\int dt \frac{d}{dt} \Leftarrow \text{total derivative}$$

$$\int_{\vec{\sigma}(t)} \vec{F}(\vec{r}) d\vec{r} = \int_{t_i}^{t_f} dt \frac{d\vec{\sigma}(t)}{dt} * \vec{F}(\vec{\sigma}(t))$$

$$\vec{\sigma}(t) = (\sigma_x(t), \sigma_y(t), \sigma_z(t))$$

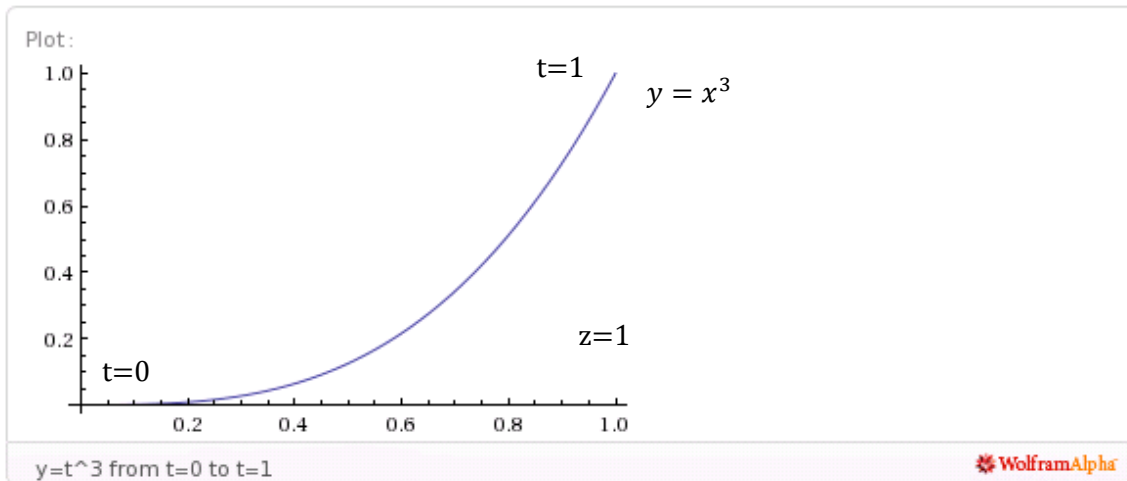
Path in 3d space

t=time, paramiterisation of path

Ex

$$\vec{F}(\vec{r}) = (x^2, z, 3x + 2y)$$

$$\vec{\sigma}(t) = (t, t^3, 1), 0 < t < 1$$

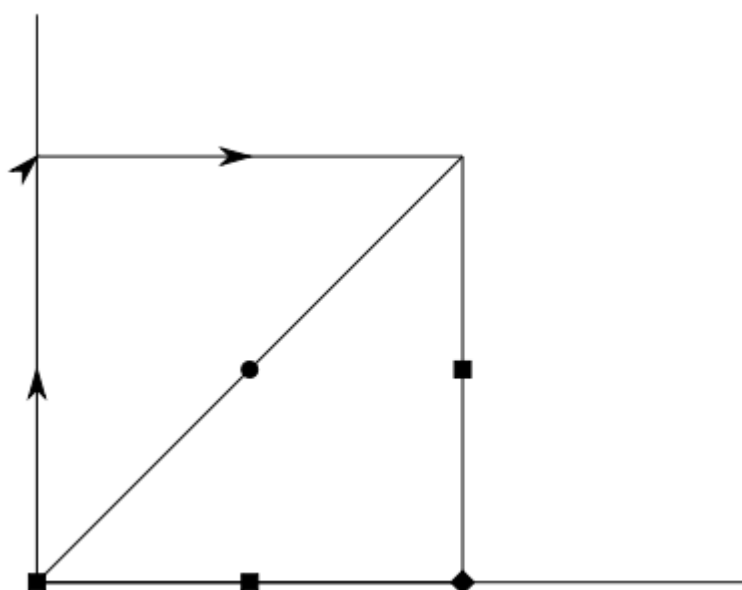


$$\int \vec{F} d\vec{r} = \int_0^1 dt \frac{d\vec{\sigma}}{dt} * \vec{F}(\vec{\sigma}(t))$$

$$\begin{aligned} \frac{d\vec{\sigma}}{dt} &= (1, 3t^2, 0) \\ \vec{F}(\vec{\sigma}(t)) &= (t^2, 1, 3t + 2t^3) \\ x &\rightarrow t, y \rightarrow t^3, z \rightarrow 1 \\ \int \frac{d\vec{\sigma}}{dt} \vec{F} &= 1 * t^2 + 3t^2 * 1 \pm (3t + 2t^3) \\ &= 4t^2 \\ \Rightarrow \int_0^1 dt 4t^2 &= \frac{4}{3} t^3 \Big|_0^1 = \frac{4}{3} \end{aligned}$$

2d example,

$$\begin{aligned} \vec{F}(x, y) &= (2xy, x^2 + axy) = (F_x, F_y) \\ c_1: &(0,0) \rightarrow (1,0) \rightarrow (1,1) \\ c_2: &(0,0) \rightarrow (1,1) \text{ along diagonal, } y=x \\ c_3: &(0,0) \rightarrow (0,1) \rightarrow (1,1) \end{aligned}$$



$$\begin{aligned} W_1 &= \int d\vec{r} * \vec{F}(x, y) = \int dx F_x(x, y) \int dy F_y(x, y) \\ \vec{F} &= (F_x, F_y), d\vec{r} = (dx, dy) \\ a(0,0) \rightarrow (1,0): & 0 < x < 1, y = 0 \Rightarrow dy = 0 \\ W_{1a} &= \int_0^1 dx F_x(x, 0) + 0 = \int_0^1 dx (2xy)_{y=0} = \int_0^1 dx 0 = 0 \\ b(1,0) \rightarrow (1,1): & x = 1, 0 < y < 1, dx = 0 \\ W_{1b} &= 0 + \int_0^1 dy F_y(1, y) = \int_0^1 dy (1 + ay) = y + \frac{1}{2} ay^2 \Big|_0^1 = 1 + \frac{a}{2} \\ W_1 &= 1 + \frac{a}{2} \end{aligned}$$

$C_2$

$$\begin{aligned} y &= x, dy = dx \\ \frac{dy}{dx} &= 1, y(x) = x \\ W_2 &= \int d\vec{r} \vec{F}(\vec{r}) = \int dx F_x(x, y) + \int dy F_y(x, y) \\ &= \int_0^1 dx F_x(x, x) + \int_0^1 dx F_y(x, x) \\ &= \int_0^1 dx (F_x(x, x) + F_y(x, x)) = \int_0^1 dx (2x^2 + x^2 + ax^2) \end{aligned}$$

$$\int_0^1 dx(3+a)x^2 = \frac{3+a}{3}x^3 \Big|_0^1$$

$$= 1 + \frac{a}{3} = W_2$$

$C_3$

$$W_{3a}: x = 0, 0 < y < 1, dx = 0$$

$$\int_0^1 dy F_y(0, y) = \int_0^1 dy 0 = 0$$

$$W_{3b}: 0 < x < 1, y = 1, dy = 0$$

$$\int_0^1 dx F_x(x, 1) = \int_0^1 dx 2x = x^2 \Big|_0^1 = 1$$

$$W_3 = 1$$

$$W_1 = 1 + \frac{a}{2}$$

$$W_2 = 1 + \frac{a}{3}$$

$$W_3 = 1$$

Work done depends on the path that is taken

$$\text{If } a = 0: W_1 = W_2 = W_3$$

$$\vec{F}(x, y) = (2xy, x^2)$$

$$\vec{F} = -\nabla\phi = \left(-\frac{\delta\phi}{\delta x}, -\frac{\delta\phi}{\delta y}\right)$$

$$\phi(x, y) = -x^2y + \text{constant}$$

$$\frac{\delta\phi}{\delta x} = -2xy = -F_x(x, y)$$

$$\frac{\delta\phi}{\delta y} = -x^2 = -F_y(x, y)$$

$\phi = \text{potential}$

When

$a \neq 0, \phi$  does not exist!

Ex

$$y^2 = x^3$$

$$y - x^{\frac{3}{2}} = x\sqrt{x}$$

$$A = (1, 1) B = (2, 2\sqrt{2})$$

$$\vec{F}(x, y) = (xy, x)$$

$$W = \int_c d\vec{r} \vec{F}(\vec{r}) = \int dt \frac{d\vec{\sigma}}{dt} * \vec{F}(\vec{\sigma}(t))$$

What is  $\vec{\sigma}(t)$ ?

$$\vec{\sigma}(t): y = t^3, x = t^2$$

$$y^2 = t^6$$

$$x^3 = t^6$$

$$\vec{\sigma}(t) = (t^2, t^3)$$

$$A = (1, 1): t = 1$$

$$B = (2, 2\sqrt{2}): t = \sqrt{2}$$

$$\frac{d\vec{\sigma}}{dt} = (2t, 3t^2)$$

$$\vec{F}(\vec{\sigma}(t)) = (t^5, t^2)$$

$$x = t^2$$

$$y = t^3$$

$$\vec{\sigma}' * \vec{F} = 2t^6 + 3t^5$$

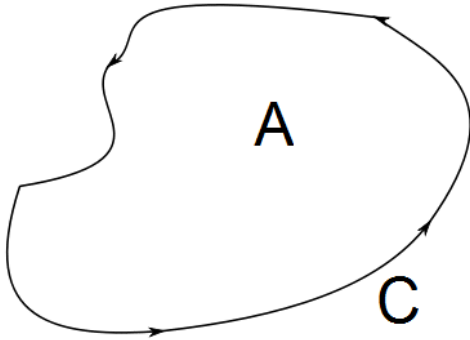
$$= 2t^6 + 3t^5$$

$$W = \int_1^{\sqrt{2}} dt (2t^6 + 3t^4) = 2/$$

Stokes theorem (2D)

$$\oint_C \vec{F} d\vec{r} = \iint_A dx dy \left( \frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} \right)$$

Sometimes LHS or RHS is easier to compute



$$\frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} = 0, \text{ then } \oint_C \vec{F} d\vec{r}$$

Vanishes for all closed contours C

Be derived from a potential  $\phi$

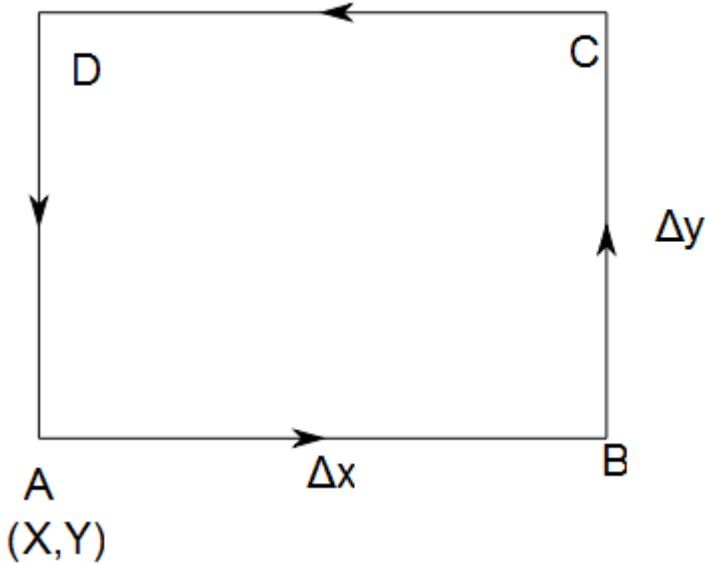
$$F_x = -\frac{\delta}{\delta x} \phi, F_y = -\frac{\delta}{\delta y} \phi$$

Then

$$\begin{aligned} & \frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} \\ &= \frac{\delta}{\delta x} \left( -\frac{\delta}{\delta y} \phi \right) - \frac{\delta}{\delta y} \left( -\frac{\delta}{\delta x} \phi \right) \\ &= \frac{\delta^2}{\delta x \delta y} \phi - \frac{\delta^2}{\delta y \delta x} \phi = 0 \end{aligned}$$

These vector fields are called conservative

Proof:



Evaluate

$$\oint_{ABCD} \vec{F} d\vec{r}$$

1.  $AB: y = Y, X < x < X + \Delta x$

$$\int_{AB} \vec{F} d\vec{r} = \int_X^{X+\Delta x} dx F_x(x, Y)$$

2.  $BC: x = X + \Delta x, Y < y < Y + \Delta y$

$$\int_{BC} \vec{F} d\vec{r} = \int_Y^{Y+\Delta y} dy F_y(X + \Delta x, y)$$

3.  $CD: X + \Delta x > x > X, y = Y + \Delta y$

$$\int_{CD} \vec{F} d\vec{r} = \int_{X+\Delta x}^X dx F_x(x, Y + \Delta y)$$

4.  $DA: Y + \Delta y > y > Y, x = X$

$$\int_{DA} \vec{F} d\vec{r} = \int_{Y+\Delta y}^Y dy F_y(X, y)$$

so

$$\begin{aligned} \oint \vec{F} d\vec{r} &= \int_{AB} \vec{F} d\vec{r} + \int_{BC} \vec{F} d\vec{r} + \int_{CD} \vec{F} d\vec{r} + \int_{DA} \vec{F} d\vec{r} \\ &= \int_X^{X+\Delta x} (F_x(x, Y) - F_x(x, Y + \Delta y)) dx + \int_Y^{Y+\Delta y} (F_y(X + \Delta x, y) - F_y(X, y)) dy \end{aligned}$$

Use  $\Delta x, \Delta y \ll 1$ , use

$$\int_X^{X+\Delta x} dx f(x) \approx f(X) \Delta x$$

$$\Rightarrow [F_x(X, Y) - F_x(X, Y + \Delta y)] \Delta x + [F_y(X + \Delta x, Y) - F_y(X, Y)] \Delta y$$

Derivative

$$\frac{df(x)}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

$$\Rightarrow -\frac{\delta}{\delta y} F_x(X, Y) \Delta y \Delta x + \frac{\delta}{\delta x} F_y(X, Y) \Delta x \Delta y$$

$$\oint_{ABCD} \vec{F} d\vec{r} = \left( \frac{\delta}{\delta x} F_y - \frac{\delta}{\delta y} F_x \right) \Delta x \Delta y = \iint dx dy \left( \frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} \right)$$

$$\Delta x \Delta y = \text{area}$$

Proved for small square

General case- divide into many small squares

$$\text{area} = \sum \text{area of squares}$$

Ex

$$\vec{F}(\vec{r}) = (2xy, x^2 + axy)$$

$$W = \int_{AB} \vec{F} d\vec{r} = 1 \text{ for all paths if } a = 0$$

1) Closed contour

$$\int_A^B dx f(x) = - \int_B^A dx f(x)$$

2) Is  $\vec{F}$  conservative?

$$\vec{F} = \nabla\phi$$

$$\phi(x, y) = -x^2y + \text{constant}$$

3) Stokes

$$\oint \vec{F} d\vec{r} = \iint \left( \frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} \right) dx dy$$

$$\frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} = 2x - 2x = 0$$

$$(a=0)$$

$$\Rightarrow \text{If } \frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} = 0$$

Then

$$\oint_C \vec{F} d\vec{r} = 0 \forall C$$

And

$$\int_{AB} \vec{F} d\vec{r}$$

Depends on begin-end point, not actual contour

NOTE: every vector field

$$\vec{F} = -\nabla\phi$$

Is conservative

$$\frac{\delta}{\delta x} F_y - \frac{\delta}{\delta y} F_x = \frac{\delta}{\delta x} \left( -\frac{\delta}{\delta y} \phi \right) - \frac{\delta}{\delta y} \left( -\frac{\delta}{\delta x} \phi \right) = 0$$

### Conservative Force Fields (2D)

$\vec{F}(\vec{r})$  is conservative:

- $\frac{\delta F_x}{\delta y} = \frac{\delta F_y}{\delta x}$
- $\vec{F}(\vec{r}) = \nabla\phi(\vec{r})$

Or

$$F_x(\vec{r}) = -\frac{\delta}{\delta x} \phi(\vec{r})$$

$$F_y(\vec{r}) = -\frac{\delta}{\delta y} \phi(\vec{r})$$

- $\oint_C \vec{F}(\vec{r}) d\vec{r} = 0$

Follows from stoke's theorem

$$\oint_C \vec{F}(\vec{r}) d\vec{r} = \iint dx dy \left( \frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} \right)$$

- $\int_{AB} \vec{F}(\vec{r}) d\vec{r}$

Depend only on begin and end points, not actual contour

$$\int_{c_1+c_2} \vec{F} d\vec{r} = 0$$

$$\int_{c_1} \vec{F} d\vec{r} + \int_{c_2} \vec{F} d\vec{r} = 0$$

$$\int_{c_1} \vec{F} d\vec{r} = - \int_{-c_2} \vec{F} d\vec{r}$$

3D

$$\vec{F}(x, y, z) = (F_x(\vec{r}), F_y(\vec{r}), F_z(\vec{r}))$$

Scalar potential

$$\phi(F) = \phi(x, y, z)$$

If  $\vec{F}(\vec{r}) = -\nabla\phi$

$$F_x = -\frac{\delta\phi}{\delta x}$$

$$F_y = -\frac{\delta\phi}{\delta y}$$

$$F_z = -\frac{\delta\phi}{\delta z}$$

Then  $\vec{F}$  is conservative

Cross product

$$\vec{F} \text{ is conservative} \Leftrightarrow \nabla \times \vec{F} = 0$$

$\nabla$ =nabla operator

Vector

$$\nabla = \left( \frac{\delta}{\delta x}, \frac{\delta}{\delta y}, \frac{\delta}{\delta z} \right)$$

$\nabla \times \vec{F}$  vector, curl of  $\vec{F}$ , curl  $\vec{F}$

$$\nabla \times \vec{F} = \left( \frac{\delta}{\delta y} F_z - \frac{\delta}{\delta z} F_y, \frac{\delta}{\delta z} F_x - \frac{\delta}{\delta x} F_z, \frac{\delta}{\delta x} F_y - \frac{\delta}{\delta y} F_x \right)$$

$\nabla\phi(\vec{r}) = \text{vector}$

$$= \left( \frac{\delta\phi}{\delta x}, \frac{\delta\phi}{\delta y}, \frac{\delta\phi}{\delta z} \right)$$

Gradient of  $\phi$

Grad  $\phi$

$\nabla * \nabla = \text{scalar}$

$$\nabla^2 = \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}$$

$\nabla^2\phi$  scalar

$$= \frac{\delta^2}{\delta x^2} \phi + \frac{\delta^2}{\delta y^2} \phi + \frac{\delta^2}{\delta z^2} \phi$$

$\nabla^2\vec{F}$  vector

$$= (\nabla^2 F_x, \nabla^2 F_y, \nabla^2 F_z)$$

$\nabla \cdot \vec{F}$  scalar, divergence of  $\vec{F}$

div  $\vec{F}$

$$= \frac{\delta F_x}{\delta x} + \frac{\delta F_y}{\delta y} + \frac{\delta F_z}{\delta z}$$

$$\vec{F} \cdot \nabla = F_x \frac{\delta}{\delta x} + F_y \frac{\delta}{\delta y} + F_z \frac{\delta}{\delta z}$$

$\vec{F} \cdot \nabla\phi$  scalar

$\vec{F} \cdot \nabla\vec{A}$  vector

$$= (\vec{F} \cdot \nabla A_x, \vec{F} \cdot \nabla A_y, \vec{F} \cdot \nabla A_z)$$

Ex

$$\phi(\vec{r}) = -\frac{1}{2}x^2y^2z^2 - 2xy + 3$$

$$\vec{F} = -\nabla\phi$$

$$F_x = -\frac{\delta\phi}{\delta x} = xy^2z^2 + 2y$$

$$F_y = -\frac{\delta\phi}{\delta y} = x^2yz^2 + 2x$$

$$F_z = -\frac{\delta\phi}{\delta z} = x^2y^2z$$

Conservative

$$\nabla \times \vec{F} = 0?$$

$$\nabla \times \vec{F} = (2x^2yz - 2x^2yz - 2xy^2z, 2xy^2z - 2xy^2z, 2xyz^2 + 2 - 2xyz^2 - 2) = (0, 0, 0)$$

$\vec{F}$  is conservative

Ex Vector field  $\vec{F}$  follows from potential  $\phi(\vec{r}) = \frac{1}{r}$

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\vec{F} = -\nabla\phi = \left( \frac{\delta\phi}{\delta x}, \frac{\delta\phi}{\delta y}, \frac{\delta\phi}{\delta z} \right)$$

$$\phi = \frac{1}{r} = \frac{1}{\sqrt{x^2 + y^2 + z^2}} = (x^2 + y^2 + z^2)^{-\frac{1}{2}}$$

$$\begin{aligned} \frac{\delta\phi}{\delta x} &= \frac{1}{2} (x^2 + y^2 + z^2)^{-\frac{3}{2}} 2x \\ &= -\frac{x}{(x^2 + y^2 + z^2)^{\frac{3}{2}}} = -\frac{x}{r^3} \end{aligned}$$

$$\frac{\delta\phi}{\delta y} = -\frac{y}{r^3}$$

$$\frac{\delta\phi}{\delta z} = -\frac{z}{r^3}$$

$$\begin{aligned} \vec{F} &= -\nabla\phi \\ &= \left( \frac{x}{r^3}, \frac{y}{r^3}, \frac{z}{r^3} \right) \\ \vec{r} &= (x, y, z) \\ &= \frac{\vec{r}}{r} = \frac{1}{r^2} \hat{r} \\ \hat{r} &= \frac{\vec{r}}{r} = \text{unit vector} \\ \hat{r} \cdot \hat{r} &= 1 \end{aligned}$$

$$\vec{F} = \frac{1}{r^2} \hat{r}$$

Strength drops as  $\frac{1}{r^2}$

Points in the radial direction

Newton gravity

Coulomb, EM

$\phi$  is constant on spheres with fixed radius

$\vec{F}$  is perpendicular to the equipotential surface

General statement

$\vec{F} \perp$  surface of constant potential

$$\phi(\vec{r}) = \phi(\vec{r} + \delta\vec{r})$$

$$\delta\vec{r} \ll 1$$

$$\phi(\vec{r} + \delta\vec{r}) = \phi(\vec{r}) + \delta\vec{r} \cdot \nabla\phi(\vec{r}) + \theta(\delta r^2)$$

$$f(x + \Delta x) = f(x) + \Delta x f'(x) + \theta(\Delta x^2)$$

$$\delta\vec{r} = (\delta x, \delta y, \delta z)$$

$$\delta x \frac{\delta\phi}{\delta x} + \delta y \frac{\delta\phi}{\delta y} + \delta z \frac{\delta\phi}{\delta z}$$

$$\phi(\vec{r} + \delta\vec{r}) = \phi(\vec{r}) + \delta\vec{r} \cdot \nabla\phi + \dots$$

But

$$\phi(\vec{r} + \delta\vec{r}) = \phi(\vec{r})$$

Since equipotential surface

$$\Rightarrow \delta\vec{r} \cdot \nabla\phi = 0 \Rightarrow \delta\vec{r} \cdot \vec{F}(\vec{r}) = 0$$

$$\Rightarrow \delta\vec{r} \perp \vec{F}(\vec{r})$$

Stokes theorem (3D)

2D:

$$\oint_C \vec{F} d\vec{r} = \iint_A dx dy \left( \frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} \right)$$

$$\left( \frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} \right) = \text{3rd component of } \nabla \times \vec{F}$$

$$= (\nabla \times \vec{F})_z$$

Normal vector of surface

$\hat{n}$

$\hat{n}$  is always  $\perp$  to surface,  $\hat{n} \cdot \hat{n} = 1$



Surface is in xy-plane  $\hat{n} = \hat{z} = (0,0,1)$

$$(\nabla \times \bar{F})_z = (\nabla \times \bar{F}) \cdot \hat{n}$$

$$\hat{n} dx dy = \hat{n} dS = d\bar{S}$$

3D

$$\oint_C \bar{F} d\bar{r} =$$

$$\iint d\bar{S} \cdot (\nabla \times \bar{F})$$

### Conservative Force Fields (2D)

$\vec{F}(\vec{r})$  is conservative:

- $\frac{\delta F_x}{\delta y} = \frac{\delta F_y}{\delta x}$
- $\vec{F}(\vec{r}) = -\nabla\phi(\vec{r})$

Or

$$F_x(\vec{r}) = -\frac{\delta}{\delta x}\phi(\vec{r})$$

$$F_y(\vec{r}) = -\frac{\delta}{\delta y}\phi(\vec{r})$$

- $\oint_c \vec{F}(\vec{r})d\vec{r} = 0$

Follows from stoke's theorem

$$\oint_c \vec{F}(\vec{r})d\vec{r} = \iint dxdy \left( \frac{\delta F_y}{\delta x} - \frac{\delta F_x}{\delta y} \right)$$

- $\int_{AB} \vec{F}(\vec{r})d\vec{r}$

Depend only on begin and end points, not actual contour

$$\int_{C_1+C_2} \vec{F}d\vec{r} = 0$$

$$\int_{C_1} \vec{F}d\vec{r} + \int_{C_2} \vec{F}d\vec{r} = 0$$

$$\int_{C_1} \vec{F}d\vec{r} = \int_{-C_2} \vec{F}d\vec{r}$$

3D

$$\vec{F}(x, y, z) = (F_x(\vec{r}), F_y(\vec{r}), F_z(\vec{r}))$$

Scalar potential

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If  $\vec{F}(\vec{r}) = -\nabla\phi$

$$F_x = -\frac{\delta\phi}{\delta x}$$

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Then  $\vec{F}$  is conservative

Cross product

$$\vec{F} \text{ is conservative } \Leftrightarrow \nabla \times \vec{F} = 0$$

$\nabla$ =nabla operator

Vector

$$\nabla = \left( \frac{\delta}{\delta x}, \frac{\delta}{\delta y}, \frac{\delta}{\delta z} \right)$$

$\nabla \times \vec{F}$  vector, curl of  $\vec{F}$ ,  $\text{curl } \vec{F}$

$$\nabla \times \vec{F} = \left( \frac{\delta}{\delta y} F_z - \frac{\delta}{\delta z} F_y, \frac{\delta}{\delta z} F_x - \frac{\delta}{\delta x} F_z, \frac{\delta}{\delta x} F_y - \frac{\delta}{\delta y} F_x \right)$$

$\nabla\phi(\vec{r}) = \text{vector}$

$$= \left( \frac{\delta\phi}{\delta x}, \frac{\delta\phi}{\delta y}, \frac{\delta\phi}{\delta z} \right)$$

Gradient of  $\phi$

$$\begin{aligned} & \text{Grad } \phi \\ \nabla \cdot \nabla &= \text{scalar} \\ \nabla^2 &= \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2} \\ \nabla^2 \phi & \text{ scalar} \\ &= \frac{\delta^2}{\delta x^2} \phi + \frac{\delta^2}{\delta y^2} \phi + \frac{\delta^2}{\delta z^2} \phi \\ \nabla^2 \bar{F} & \text{ vector} \\ &= (\nabla^2 F_x, \nabla^2 F_y, \nabla^2 F_z) \\ \nabla \cdot \bar{F} & \text{ scalar, divergence of } \bar{F} \\ \text{div } \bar{F} & \\ &= \frac{\delta F_x}{\delta x} + \frac{\delta F_y}{\delta y} + \frac{\delta F_z}{\delta z} \end{aligned}$$

$$\begin{aligned} \bar{F} \cdot \nabla &= F_x \frac{\delta}{\delta x} + F_y \frac{\delta}{\delta y} + F_z \frac{\delta}{\delta z} \\ \bar{F} \cdot \nabla \phi & \text{ scalar} \\ \bar{F} \cdot \nabla \bar{A} & \text{ vector} \\ &= (\bar{F} \nabla A_x, \bar{F} \nabla A_y, \bar{F} \nabla A_z) \end{aligned}$$

Ex

$$\begin{aligned} \phi(\vec{r}) &= -\frac{1}{2}x^2y^2z^2 - 2xy + 3 \\ \bar{F} &= -\nabla\phi \\ F_x &= -\frac{\delta\phi}{\delta x} = xy^2z^2 + 2y \\ F_y &= -\frac{\delta\phi}{\delta y} = x^2yz^2 + 2x \\ F_z &= -\frac{\delta\phi}{\delta z} = x^2y^2z \end{aligned}$$

Conservative

$$\nabla \times \bar{F} = 0?$$

$$\nabla \times \bar{F} = (2x^2yz - 2x^2yz - 2xy^2z, 2xy^2z - 2xy^2z, 2xyz^2 + 2 - 2xyz^2 - 2) = (0,0,0)$$

$\bar{F}$  is conservative

Ex Vector field  $\bar{F}$  follows from potential  $\phi(\vec{r}) = \frac{1}{r}$

$$\begin{aligned} r &= \sqrt{x^2 + y^2 + z^2} \\ \bar{F} &= -\nabla\phi = \left( \frac{\delta\phi}{\delta x}, \frac{\delta\phi}{\delta y}, \frac{\delta\phi}{\delta z} \right) \\ \phi &= \frac{1}{r} = \frac{1}{\sqrt{x^2 + y^2 + z^2}} = (x^2 + y^2 + z^2)^{-\frac{1}{2}} \\ \frac{\delta\phi}{\delta x} &= \frac{1}{2}(x^2 + y^2 + z^2)^{-\frac{3}{2}}2x \\ &= -\frac{x}{(x^2 + y^2 + z^2)^{\frac{3}{2}}} = -\frac{x}{r^3} \\ \frac{\delta\phi}{\delta y} &= -\frac{y}{r^3} \\ \frac{\delta\phi}{\delta z} &= -\frac{z}{r^3} \\ \bar{F} &= -\nabla\phi \\ &= \left( \frac{x}{r^3}, \frac{y}{r^3}, \frac{z}{r^3} \right) \\ \vec{r} &= (x, y, z) \\ &= \frac{\vec{r}}{r^3} = \frac{1}{r^2} \hat{r} \\ \hat{r} &= \frac{\vec{r}}{r} = \text{unit vector} \\ \hat{r} \cdot \hat{r} &= 1 \end{aligned}$$

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$$\delta\vec{r} = (\delta x, \delta y, \delta z)$$

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$$\oint_C \vec{F} d\vec{r} = \iint_A (\nabla \times \vec{F})_z$$

$$\iint_A (\nabla \times \vec{F})_z$$

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Eg. Surface is in xy-plane  $\hat{n} = \hat{z} = (0,0,1)$

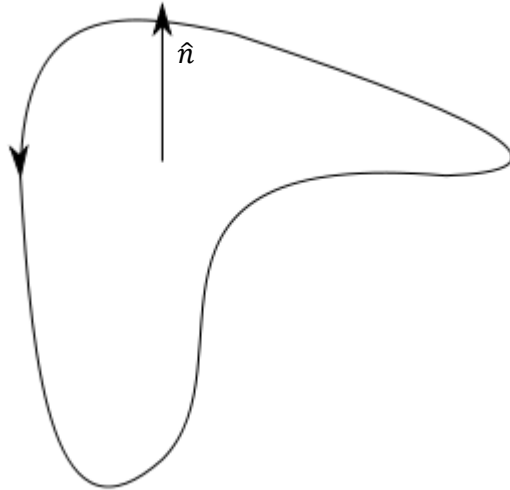
Eg. Sphere:  $\hat{n} = \hat{r} = \frac{\vec{r}}{r} = \left( \frac{x}{r}, \frac{y}{r}, \frac{z}{r} \right)$

$$(\nabla \times \vec{F})_z = (\nabla \times \vec{F}) \cdot \hat{n}$$

$$\hat{n} dx dy = \hat{n} dS = d\vec{S}$$

If surface is closed (sphere) then  $\hat{n}$  points outwards

If surface is open, i.e. it has a boundary, then the direction of the normal vector follows from Right hand rule



Surface is characterised by

Area

Normal vector

$$\iint d\vec{S} = \iint \hat{n} dS$$

$dS=2D$  integral

$$\oint \vec{F} d\vec{r} = \iint dx dy (\nabla \times \vec{F})_z$$

$$\hat{n} = (0,0,1)$$

$$Dx dy = dS$$

$$(\nabla \times \vec{F})_z = \hat{n} (\nabla \times \vec{F})$$

$$= \iint dS \hat{n} (\nabla \times \vec{F}) = \iint dS (\nabla \times \vec{F})$$

3D

$$\oint_C \vec{F} d\vec{r} =$$

$$\iint_A d\vec{S} * (\nabla \times \vec{F})$$

Ex HEMISPHERE

$$x^2 + y^2 + z^2 = a^2$$

$$z > 0$$

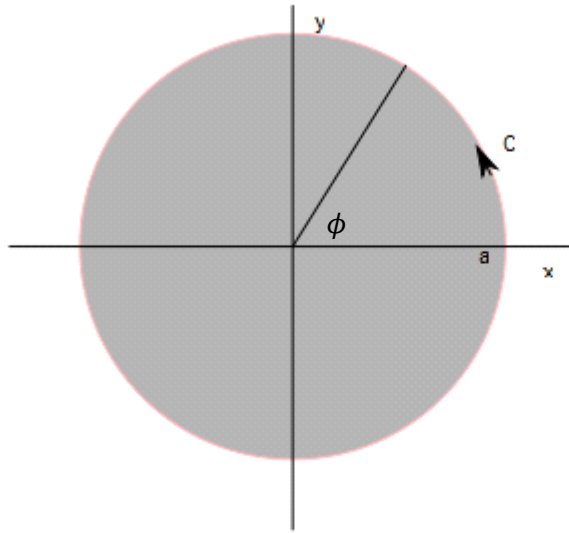
Boundary C

$$x^2 + y^2 = a^2, z = 0$$

$$\vec{F}(\vec{r}) = (-y, x, 0)$$

Verify Stokes theorem

- $\oint_C \vec{F} d\vec{r}$



$$\oint_C \vec{F}(\vec{r}) d\vec{r} = \int_0^{2\pi} d\phi \frac{d\vec{r}}{d\phi} \vec{F}(\vec{r}(\phi)) = \int_0^{2\pi} d\phi a^2 = 2\pi a^2$$

$$\frac{d\vec{r}}{d\phi} = \text{jacobian}$$

$$\frac{d\vec{r}}{d\phi} = \left( \frac{dx}{d\phi}, \frac{dy}{d\phi}, \frac{dz}{d\phi} \right)$$

$$= (-a \sin \phi, a \cos \phi, 0)$$

$$\vec{F}(\vec{r}(\phi)) = (-a \sin \phi, a \cos \phi, 0)$$

$$\frac{d\vec{r}}{d\phi} * \vec{F} = a^2 \sin^2 \phi + a^2 \cos^2 \phi + 0 = a^2$$

2.  $\iint d\vec{S} * \nabla \times \vec{F}$

$$\hat{n} = \hat{r} = \frac{\vec{r}}{r} = \frac{r}{a}$$

$$= \left( \frac{x}{a}, \frac{y}{a}, \frac{z}{a} \right)$$

$$\vec{F} = (-y, x, 0)$$

$$\nabla \times \vec{F} = (\delta_y F_z - \delta_z F_y, \delta_z F_x - \delta_x F_z, \delta_x F_y - \delta_y F_x)$$

$$= (0 - 0, 0 - 0, 1 - -1)$$

$$= (0, 0, 2)$$

$$\iint d\vec{S} * \nabla \times \vec{F} = \iint dS \hat{n} \nabla \times \vec{F}$$

$$x = a \cos \phi \sin \theta$$

$$y = a \sin \phi \sin \theta$$

$$z = a \cos \theta$$

$$0 < \phi < 2\pi$$

$$0 < \theta < \frac{\pi}{2}$$

Upper hemisphere

$$\hat{n} \nabla \times \vec{F} = \frac{\vec{r}}{a} * (0, 0, 2) = \frac{2z}{a} = \frac{2a \cos \theta}{a} = 2 \cos \theta$$

$$\text{Jacobian} = r^2 \sin \theta = a^2 \sin \theta$$

$$= \int_0^{\frac{\pi}{2}} d\theta \int_0^{2\pi} a^2 \sin \theta 2 \cos \theta$$

$$= a^2 \int_0^{2\pi} d\phi \int_0^{\frac{\pi}{2}} d\theta 2 \sin \theta \cos \theta = a^2 \int_0^{2\pi} d\phi \int_0^{\frac{\pi}{2}} d\theta \sin 2\theta$$

$$= 2\pi a^2 \left[ -\frac{1}{2} \cos 2\theta \right]_0^{\frac{\pi}{2}}$$

$$= 2\pi a^2 \left(-\frac{1}{2}\right) (-1 - 1) = 2\pi a^2$$

Integrals of the type

$$\iint \vec{F} d\vec{S}$$

Flux of  $\vec{F}$  through surface S

$$Q = \iint \vec{E} d\vec{S}$$

Electromagnetism

$$\vec{F} = (0, 0, x^2 + y^2)$$

Plane  $x=2$

Flux=0 since  $\vec{F} // \text{plane}$   $\vec{F} \perp \hat{n}$

Plane  $z=2$

Flux  $\neq 0$

$$\vec{F} \perp \text{plane}$$

$$\vec{F} // \hat{n}$$

Ex

Surface is closed box with side length a

Vector field  $\vec{F} = (x, y, z) = \hat{r}$

Consider each side separately

1. Front

$$x = a, 0 < y, z < a$$

$$\hat{n} = (1, 0, 0)$$

$$\iint d\vec{S} \vec{F} = \iint dS \hat{n} * \vec{F}$$

$$= \int_0^a dy \int_0^a dz F_x(a, y, z)$$

$$= \int_0^a dy \int_0^a dz x \Big|_{x=a}$$

$$= a^3$$

2. Back

$$x = 0, 0 < y, z < a$$

$$\hat{n} = (-1, 0, 0)$$

$$\hat{n} \vec{F} = -F_x(0, y, z)$$

$$= -x \Big|_{x=0} = 0$$

3. Top

$$z = a, 0 < x, y < a$$

$$\hat{n} = (0, 0, 1)$$

$$\hat{n} \vec{F} = F_z(x, y, a)$$

$$= a$$

$$\int_0^a dx \int_0^a dy a = a^3$$

4. Bottom,  $z=0$

$$\hat{n} = (0, 0, -1)$$

$$\hat{n} \vec{F} = -F_z(x, y, 0)$$

$$= 0$$

5. Left side,  $y=0$

$$\hat{n} = (0, -1, 0)$$

$$\hat{n} \vec{F} = -F_y(x, 0, z) = 0$$

6. Right side

$$y = a$$

$$\hat{n} = (0, 1, 0)$$

$$\hat{n} \vec{F} = F_y(x, a, z)$$

$$\int_0^a dx \int_0^a dz F_y(x, a, z)$$

$$= a^3$$

# Divergence Theorem

13 December 2011

11:04

(Gauss theorem)

Consider a closed surface  $S$  in  $\mathbb{R}^3$

3D interior volume  $V$

$$S = \partial V$$

Consider a vector field  $\vec{F}(\vec{r})$

$$\iint \vec{F}(\vec{r}) d\vec{S} = \iiint \nabla \cdot \vec{F}(\vec{r}) dV$$

Flux through surface = Volume integral of  $\text{div } \vec{F}$

Proof

Consider a small cube and compute both sides using  $\Delta x, \Delta y, \Delta z \ll 1$

We have already computed the flux (see notes)

Flux through left, bottom, back = 0, follows from symmetry

Right, front, top: Flux =  $a^3$

$$\begin{matrix} (a^2 & * & a) \\ \text{Area} & & \vec{F} \Big|_{\text{sides}} \end{matrix}$$

$$\Rightarrow \text{total flux } 3a^3$$

Div theorem

$$\begin{aligned} \nabla \cdot \vec{F} &= \frac{\partial}{\partial x} F_x + \frac{\partial}{\partial y} F_y + \frac{\partial}{\partial z} F_z, \vec{F} = \vec{r} = (x, y, z) \\ &= 1 + 1 + 1 = 3 \end{aligned}$$

$$\iiint_{\text{cube}} \nabla \cdot \vec{F} dV = 3 \iiint_{\text{cube}} dV = 3a^3$$

Ex sphere,  $\vec{F}(\vec{r}) = \vec{r}$

$$\iint \vec{F} \cdot d\vec{S}$$

$$d\vec{S} = \hat{n} dS$$

$$\hat{n} = \hat{r} = \frac{\vec{r}}{r}$$

$$dS = a^2 \sin \theta d\phi d\theta$$

$$a^2 \sin \theta = \text{jacobian} \Big|_{r=a}$$

$$\iint \vec{F} \cdot d\vec{S} = \int_0^{2\pi} d\phi \int_0^\pi d\theta a^2 \sin \theta a$$

$$= a^3 2\pi \int_0^\pi d\theta \sin \theta$$

$$= a^3 2\pi [-\cos \theta]_0^\pi$$

$$= 4\pi a^3$$

$$\iiint_{\text{sphere}} \nabla \cdot \vec{F} dV, \nabla \cdot \vec{F} = 3$$

$$= 3 \iiint_{\text{sphere}} dV = 3 \frac{4\pi}{3} a^3 = 4\pi a^3$$

Ex

$$\iint (x^2 + y + z) dS$$

$S$  = closed surface of sphere, radius 1

$$x^2 + y^2 + z^2 = r^2 = 1$$

Use Gauss' theorem!

$$\iint \vec{F} \cdot d\vec{S} = \iiint \nabla \cdot \vec{F} dV$$

Find  $\vec{F}$  such that  $\iint \vec{F} \cdot d\vec{S} = \iint (x^2 + y + z) dS$

$$d\vec{S} = \hat{n} dS, \hat{n} = \hat{r} = \left( \frac{x}{r}, \frac{y}{r}, \frac{z}{r} \right)$$

$$\vec{F} \cdot \hat{n} = x^2 + y + z$$



$$F_x \frac{x}{r} + F_y \frac{y}{r} + F_z \frac{z}{r} \Big|_{r=1} = x^2 + y + z$$

$$F_x x + F_y y + F_z z = x^2 + y + z$$

$$F_x = x$$

$$\rightarrow F_y = F_z = 1$$

$$\vec{F}(\vec{r}) = (x, 1, 1)$$

Now RHS

$$\nabla \cdot \vec{F} = \frac{\delta}{\delta x} x + \frac{\delta}{\delta y} 1 + \frac{\delta}{\delta z} 1 = 1$$

$$\iiint_{\text{sphere}} \nabla \cdot \vec{F} dV = \iiint_{\text{sphere}} dV = \frac{4\pi}{3}$$

### Recap of integral theorems

Ordinary integration

$$I = \int_a^b dx f(x), f(x) = \frac{dg(x)}{dx}$$

g(x) = primitive

$$[= g(x)]_a^b = g(b) - g(a)$$

-end points

"surface terms" boundary

Conservative vector field  $\vec{F}(\vec{r})$

$$\Leftrightarrow \nabla \times \vec{F} = \vec{0}$$

$$\Leftrightarrow \vec{F} = -\nabla\phi$$

$\phi$  is a potential

$$I = \int_a^b \vec{F} d\vec{r} = - \int_a^b d\vec{r} \nabla\phi$$

$$= -(\phi(B) - \phi(A))$$

"surface term" boundaries

Work done = difference in potential energy

Stokes' theorem

2D:

$$\iint_A \left( \frac{\delta}{\delta x} F_y - \frac{\delta}{\delta y} F_x \right) dx dy = \oint_C \vec{F}(\vec{r}) d\vec{r}$$

3D:

$$\iint_A (\nabla \times \vec{F}) \cdot d\vec{S} = \oint_C \vec{F} d\vec{r}$$

A = area, C = boundary "surface term",  $\nabla \times \vec{F}$  = "derivative"

Divergence theorem

$$\iiint_V \nabla \cdot \vec{F} dV = \iint_S \vec{F} d\vec{S}$$

Boundary

$$S = \delta V$$

REVISION CLASS Fri 13/1 Glyn E

$$1) \int_{\bar{\sigma}(\phi)} \bar{F}(\bar{r}) \cdot d\bar{r}$$

$$\bar{F}(\bar{r}) = (-xy, x^2)$$

$$\bar{\sigma}(\phi) = (\cos \phi, \sin \phi)$$

$$0 < \phi < \frac{\pi}{2}$$

$$x = \cos \phi$$

$$y = \sin \phi$$

$$\int \bar{F}(\bar{r}) d\bar{r} = \int_0^{\frac{\pi}{2}} d\phi \frac{d\bar{\sigma}}{d\phi} \bar{F}(\bar{\sigma}(\phi))$$

$$1. \frac{d\bar{\sigma}}{d\phi} = (-\sin \phi, \cos \phi)$$

$$x = \sigma_x(\phi) = \cos \phi$$

$$y = \sigma_y(\phi) = \sin \phi$$

$$2. \bar{F}(\bar{\sigma}(\phi)) = (-\cos \phi \sin \phi, \cos^2 \phi)$$

$$3. \frac{d\bar{\sigma}}{d\phi} \bar{F} = c\phi s^2\phi + c^2\phi$$

$$c\phi(s^2\phi c^2\phi) = c\phi$$

$$4. \int_0^{\frac{\pi}{2}} d\phi c\phi = s\phi \Big|_0^{\frac{\pi}{2}} = 1$$

$$2) \bar{A}(\bar{r}) = (xyz^2 + x^2, y + xz, z^2)$$

$$1. \bar{A} \cdot \bar{A} \text{ scalar}$$

$$= A_x^2 + A_y^2 + A_z^2$$

$$2. \nabla \cdot \bar{A} = \text{div } \bar{A}$$

$$\nabla = \text{nabla}$$

$$= \left( \frac{\delta}{\delta x}, \frac{\delta}{\delta y}, \frac{\delta}{\delta z} \right)$$

$$\nabla \cdot \bar{A} = \frac{\delta}{\delta x} A_x + \frac{\delta}{\delta y} A_y + \frac{\delta}{\delta z} A_z$$

$$= yz^2 + 2x + 1 + 2z$$

$$3. \nabla(\nabla \cdot \bar{A}) \text{ grad div } \bar{A}$$

$$\nabla \cdot \bar{A} = \phi$$

$$\nabla \phi \text{ vector}$$

$$= \left( \frac{\delta}{\delta x} \phi, \frac{\delta}{\delta y} \phi, \frac{\delta}{\delta z} \phi \right)$$

$$= (2, z^2, 2yz + 2)$$

$$4. \nabla^2 \bar{A} \text{ vector}$$

$$\nabla^2 = \nabla * \nabla \text{ scalar}$$

$$= \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}$$

$$= (\nabla^2 A_x, \nabla^2 A_y, \nabla^2 A_z)$$

$$= (2 + 0 + 2xy, 0 + 0 + 0, 0 + 0 + 2)$$

$$\nabla(\nabla \cdot \bar{A}) = \bar{w}$$

$$\nabla_j \nabla_i A_i = w_j$$

$$\nabla^2 \bar{A} = \bar{w}$$

$$\nabla_i \nabla_i A_j = w_j$$

$$5. \nabla \times \bar{A} =$$

$$(\delta_y A_z - \delta_z A_y, \delta_z A_x - \delta_x A_z, \delta_x A_y - \delta_y A_x)$$

$$6. \nabla * \nabla \times \bar{A} = \nabla * \bar{B}$$

Scalar

$$= -1 + 2xz + 1 - 2xz$$

$$= 0$$

Not surprise

$$\bar{a} \times \bar{b} = \bar{c}$$

$$\bar{a} \cdot \bar{b} \times \bar{c} = \bar{c} \cdot \bar{a} \times \bar{b} = \bar{b} \cdot \bar{c} \times \bar{a}$$

Cyclic

$$\bar{a} \cdot \bar{a} \times \bar{b} = \bar{b} \cdot \bar{a} \times \bar{a}$$

$$\bar{a} \times \bar{b} = \bar{c} \perp \bar{a}$$

$$\bar{a} \cdot \bar{c} = 0$$

$$\bar{A} \cdot \nabla \bar{A} = \bar{H}$$

$$\bar{A} * \nabla = A_x \frac{\delta}{\delta x} + A_y \frac{\delta}{\delta y} + A_z \frac{\delta}{\delta z}$$

$$\neq \bar{A} \nabla \cdot \bar{A}$$

$$\nabla \cdot \bar{A} = \text{div } \bar{A}$$

$$\bar{A} * \nabla = \bar{H} = (\bar{A} \nabla A_x, \bar{A} \nabla A_y, \bar{A} \nabla A_z)$$

$$3) \bar{F}(\bar{r}) = (3x^2y^2z, 2x^3yz, x^3y^2)$$

$$\frac{d\bar{\sigma}}{dt} = (1, 2t, 3t^2)$$

$$\bar{F}(\bar{\sigma}(t))$$

$$x = t$$

$$y = t^2$$

$$z = t^3$$

1. Conservative

$$\nabla \times \bar{F} = (0, 0, 0)$$

2.  $\phi$  scalar, 2 function

$$\bar{F} = -\nabla \phi$$

$$F_x = -\frac{\delta}{\delta x} \phi = x^2y^2z \quad (1)$$

$$F_y = -\frac{\delta}{\delta y} \phi = 2x^3yz \quad (2)$$

$$F_z = -\frac{\delta}{\delta z} \phi = x^3y^2 \quad (3)$$

$$(1) \frac{\delta \phi}{\delta x} = -3x^2y^2z$$

$$(2) \frac{\delta \phi}{\delta y} = -2x^3yz$$

$$(3) \frac{\delta \phi}{\delta z} = -x^3y^2$$

$$\phi(x, y, z) = -x^3y^2z + f(y, z)$$

$$\phi(x, y, z) = -x^3y^2z + g(x, z)$$

$$\phi(x, y, z) = -x^3y^2z + h(x, y)$$

$$\phi(x, y, z) = x^3y^2z + c$$

$$3. \int_{\bar{\sigma}(t)} \bar{F}(\bar{r}) d\bar{r}$$

$$0 < t < 1$$

$$\bar{\sigma}(t) = (t, t^2, t^3)$$

$$\int_0^1 dt \frac{d\bar{\sigma}}{dt} \cdot \bar{F}(\bar{\sigma}(t))$$

$$F(\bar{\sigma}(t)) = (3t^9, 2t^8, t^7)$$

$$\frac{d\bar{\sigma}}{dt} \cdot \bar{F} = 3t^9 + 4t^9 + 3t^9 = 10t^9$$

$$\int_0^1 dt 10t^9 = t^{10} \Big|_0^1 = 1$$

4)  $\vec{G}(\vec{r}) = (x^2y, xy)$

1.  $y = x$   $(0,0) \rightarrow (1,1)$

$$\vec{\sigma}(t) = (t, t)$$

$$0 < t < 1$$

$$\int d\vec{r} \vec{G}(\vec{r}) =$$

# Hamiltonian systems

04 October 2011

13:02

1. Phase space  $\Gamma$
2. Hamiltonian  $H: \Gamma \rightarrow \mathbb{R}$
3. Equations of motion  $\begin{cases} \dot{q} = \frac{\delta H}{\delta p} \\ \dot{p} = -\frac{\delta H}{\delta q} \end{cases}$
4. Boundary conditions  $\begin{cases} q(0) = q_0 \\ p(0) = p_0 \end{cases}$

Example 2: harmonic oscillator

- Lagrangian

$$L = \frac{1}{2} m \dot{q}^2 - \frac{1}{2} m \omega^2 q^2$$
$$E.o.m.: 0 = \frac{\delta}{\delta q} L - \frac{d}{dt} \left( \frac{\delta L}{\delta \dot{q}} \right)$$
$$= -m\omega^2 q - m\ddot{q}$$
$$\boxed{\ddot{q} = -\omega^2 q}$$

- Newtonian mechanics

$$F = ma$$
$$F = -kq$$
$$m\ddot{q} = -kq$$
$$\Rightarrow \ddot{q} = -\omega^2 q$$
$$\omega^2 \equiv \frac{k}{m}$$

- Hamiltonian case

$$H = \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 q^2$$

(total energy!)

$$e.o.m.: \dot{q} = \frac{\delta H}{\delta p} = \frac{p}{m}$$
$$\dot{p} = -\frac{\delta H}{\delta q} = -m\omega^2 q$$

Time derivative of first

$$\ddot{q} = \frac{\dot{p}}{m} = -\omega^2 q$$

Legendre transform

Formal technique, allowing to reformulate problems in equivalent ways

Def: start from lagrangian eg  $L = \frac{1}{2} m \dot{q}^2 - V(q)$   $L(q, \dot{q})$

Define momentum  $p \equiv \frac{\delta L}{\delta \dot{q}} = m\dot{q}$

Define  $H = \dot{q}p - L$

$$= \frac{1}{2m} p^2 + V(q)$$

# Thermodynamics

06 October 2011

13:22

Thermodynamic system: any macroscopic system

Thermodynamic parameters : V,T,P,N,... things that can be measured w/o disrupting system

Thermodynamic state: specify parameters

Thermodynamic equilibrium: no time dependence

Equation of state: functional relation among parameters

Thermodynamic transformation: change of state

Quasi-static: intermediate steps equilibrium

Reversible: quasi static, goes through same steps on way back

Work W: from mechanics

Heat Q: thing exchanged when temperature changes without producing work

Heat capacity:  $C = \frac{\Delta Q}{\Delta T}$

Heat reservoir: very big system, such that  $C \rightarrow \infty$

Ideal gas: limiting case of a diluted gas

N identical particles

Point-like particles

Interactions short range

## State function

Any function which depends on the state occupied by the system (parameters) but not on the history of the system

1. U(internal energy), S(entropy) are state functions

$$2. \int_{\gamma} du = 0 = \int_{\gamma} ds$$

Where  $\gamma$  is a closed path in the space of parameters

3.  $dU$  and  $dS$  are exact differentials (it is NOT true for W, Q)

4. U, S defined (classically) up to a constant

Thermodynamic potential

Helmoltz free energy

$$F \equiv U - TS$$

Gibbs free energy

$$G \equiv F + PV$$

Enthalpy

$$H \equiv U + PV$$

## Digression: differentiating functions of many variables

12 October 2011

09:07

$$f: \mathbb{R}^m \rightarrow \mathbb{R}$$

Differential

$$df = \left(\frac{\delta f}{\delta x_1}\right) dx_1 + \left(\frac{\delta f}{\delta x_2}\right) dx_2 + \dots$$

Partial derivatives

$$\frac{\delta f}{\delta x_i}$$

$$\delta x_i$$

$$f(x_1 + x_2 + \dots + x_m)$$

"vector"

$$\left(\frac{\delta f}{\delta x_1}, \frac{\delta f}{\delta x_2}, \dots\right)$$

Second differential is  $m \times m$  matrix

It is a symmetric matrix

$$\frac{\delta^2 f}{\delta x_i \delta x_j} = \frac{\delta^2 f}{\delta x_j \delta x_i}$$

### ★ 1st law thermodynamics

The quantity  $dU \equiv \delta Q - \delta W$  (conventional!)

Is an exact differential and it defines the state function U (internal energy)

### ★ 2nd law thermodynamics

The quantity

$$dS \equiv \frac{\delta Q}{T}$$

Is exact diff. for reversible infinitesimal transformations and defines a state function S (entropy)

Also: the entropy of a thermally isolated system is non-decreasing (clausius theorem)

### ★ 3rd law thermodynamics

The entropy S at  $T \rightarrow 0$  is universal (=does not depend on the system) and can be chosen to vanish

$$S(T \rightarrow 0) = 0$$

Exercise: internal energy of ideal gas

1. dU and dS exact
2. Eq. of state  $PV = NkT$

Show that  $U = U(T)$

Depends only on T

$$U = \frac{3}{2} NkT$$

Proof:

$$\begin{aligned} \text{1st law: } \delta Q &= dU + \delta W \\ \delta W &= P dV \end{aligned}$$

$$\text{2nd law: } \delta Q = T ds$$

$$\delta Q = \frac{\delta U}{\delta T} + \frac{\delta U}{\delta V} dV + P dV$$

Assuming that  $U=U(V,T)$

$$dS = \frac{1}{T} \left( \frac{\delta U}{\delta T} \right) dT + \frac{1}{T} \left( \frac{\delta U}{\delta V} + P \right) dV$$

$$\frac{\delta}{\delta V} \left[ \frac{1}{T} \frac{\delta U}{\delta T} \right] = \frac{\delta}{\delta T} \left[ \frac{1}{T} \left( \frac{\delta U}{\delta V} + P \right) \right]$$

From the fact that the matrix of second derivatives is symmetric

"who got lost?"  
Most of class raises  
hand  
"very good"

$$\begin{aligned} &\text{if } U = U(V, T), \\ &\text{by definition} \\ dU &= \frac{\delta U}{\delta V} dV + \frac{\delta U}{\delta T} dT \end{aligned}$$

$$\frac{1}{T} \left( \frac{\delta U}{\delta T} \right) dT \Rightarrow \frac{\delta S}{\delta T}$$

$$\frac{1}{T} \left( \frac{\delta U}{\delta V} + P \right) dV \Rightarrow \frac{\delta S}{\delta V}$$

$$\frac{\delta}{\delta V} \left[ \frac{1}{T} \frac{\delta U}{\delta T} \right] \Rightarrow \frac{\delta}{\delta V} \frac{\delta}{\delta T} S$$

$$\frac{\delta}{\delta T} \left[ \frac{1}{T} \left( \frac{\delta U}{\delta V} + P \right) \right] \Rightarrow \frac{\delta}{\delta T} \frac{\delta}{\delta V} S$$

$$\frac{1}{T} \frac{\delta^2}{\delta V \delta T} U = \frac{1}{T} \frac{\delta^2}{\delta T \delta V} U - \frac{1}{T^2} \left( \frac{\delta U}{\delta V} + P \right) + \frac{1}{T} \frac{\delta}{\delta T} P$$

$$dU \text{ exact} \Rightarrow \frac{1}{T} \frac{\delta^2}{\delta V \delta T} U = \frac{1}{T} \frac{\delta^2}{\delta T \delta V}$$

$$0 = -\frac{1}{T^2} \frac{\delta U}{\delta V} - \frac{P}{T^2} + \frac{1}{T} \frac{\delta P}{\delta T}$$

$$PV = NkT$$

$$\boxed{P = \frac{NkT}{V}}$$

$$\frac{\delta P}{\delta T} = \frac{\delta}{\delta T} \left( \frac{NkT}{V} \right) = \frac{Nk}{V}$$

$$T \frac{\delta P}{\delta T} = \frac{NkT}{V} = P$$

$$0 = \frac{1}{T^2} \left( -\frac{\delta U}{\delta V} - P + T \frac{\delta P}{\delta T} \right)$$

$$0 = \frac{1}{T^2} \left( -\frac{\delta U}{\delta V} - P + P \right) \Rightarrow 0 = \frac{1}{T^2} \left( -\frac{\delta U}{\delta V} \right)$$

$$T \neq 0 \Rightarrow \boxed{\frac{\delta U}{\delta V} = 0}$$

Maxwell Relations

Set 1:  $dU = \delta Q - \delta W$  (1st law)

$$= TdS - PdV \text{ (2nd law)}$$

$$T = \left( \frac{\delta U}{\delta S} \right)_V$$

$$P = - \left( \frac{\delta U}{\delta S} \right)_S$$

It is natural to write U as a function U(S,V) of S,V

$\delta Q$ : infinitesimal amount of heat given to a system

$\delta W$  infinitesimal amount of work done by a system

Set 2: Helmholtz Free Energy

$$F \equiv U - TS$$

Differentiate

$$dF = dU - d(TS)$$

$$= dU - SdT - TdS$$

$$= TdS - PdV - SdT - TdS$$

$$\boxed{dF = -PdV - SdT}$$

$$\Rightarrow F = F(T, V)$$

$$S = - \left( \frac{\delta F}{\delta T} \right)_V$$

$$P = - \left( \frac{\delta F}{\delta V} \right)_T$$

Set 3 Gibbs Free Energy

$$G = F + PV$$

$$dG = -SdT + VdP$$

$$S = - \left( \frac{\delta G}{\delta T} \right)_P$$

$$V = \left( \frac{\delta G}{\delta P} \right)_T$$

Set 4 Enthalpy

$$H = G + TS$$

$$dH = TdS + VdP$$

$$T = \left( \frac{\delta H}{\delta S} \right)_P$$

$$V = \left( \frac{\delta H}{\delta P} \right)_S$$

$$U(S, V) \leftrightarrow_{S-T} F(T, V)$$

$$\begin{array}{ccc} \uparrow_{P-V} & & \uparrow_{P-V} \\ H(S, P) & \leftrightarrow_{S-T} & G(T, P) \end{array}$$



Legendre Transform!  
Analogous to

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

# Classical Statistical Mechanics

13 October 2011

09:28

- We study systems
  - Large number particles  $N$
  - Occupy volume  $V$  (assumed to be finite)
  - Equilibrium!
- Basic Strategy
  - Replace/generalize the method of "most likely distribution" by sets of counting exercises and "ensemble averages"
- Input
  - Phase-space  $\Gamma$
  - Hamiltonian
  - Density function
    - Counts number of microscopic states as a function of phase-space variables
  - All physical quantities (macroscopic level) are computed as ensemble averages:

$$\langle f \rangle \equiv \frac{\int_{\Gamma} d^{3N}q d^{3N}p \rho(q_i, p_j) f(q_i, p_j)}{\int_{\Gamma} d^{3N}q d^{3N}p \rho(q_i, p_j)}$$

$f \Rightarrow$  any function

## microcanonical ensemble

Consider system isolated

1.  $N$  is fixed
2.  $E=U$  is fixed

This defines  $\rho$  to be

$$\rho = \begin{cases} 1 & \text{if } E < H < E + \Delta \\ 0 & \text{otherwise} \end{cases}$$

Where  $\Delta$  infinitesimal

## Microcanonical Ensemble

Assume system isolated

$$\begin{cases} U = E & \text{Fixed} \\ N & \text{Fixed} \end{cases}$$

$\Delta$  small energy interval ( $\Delta \ll E$ )

$$\begin{cases} 1 & \text{if } E < H < E + \Delta \\ 0 & \text{otherwise} \end{cases}$$

$$\Sigma(E) = \int_{\Gamma}^{H < E} d^{3N}q d^{3N}p$$

Volume of phase space with  $E > H$

$$d^{3N}q \equiv dq_1 dq_2 dq_3 \dots dq_{3n}$$

$$\Omega(E) \equiv \int_{\Gamma} d^{3N}q d^{3N}p \rho(p, q)$$

Volume of phase space occupied by the ensemble

$$= \int_{\Gamma} d^{3N}q d^{3N}p$$

$$E < H < E + \Delta$$

$$= \Sigma(E + \Delta) - \Sigma(E)$$

$$\omega(E) \equiv \frac{\delta \Sigma E}{\delta E} \Rightarrow \Omega(E) = \Delta \omega(E)$$

$\Delta \ll E$

$$\boxed{S(E, V, N) \equiv \kappa \ln \Omega(E)}$$

We identify  $S$  with entropy

In thermodynamics

$$dS = \frac{\delta Q}{T}$$

1. S is Extensive

(the S of a system is the sum of S for subsystems)

$$N = N_1 + N_2$$

$$V = V_1 + V_2$$

$$H = H_1 + H_2$$

↑ CAREFUL! Assumes short-range interactions

$$S(E_1, V_1, N_1) = k \ln \Omega_1(E_1)$$

$$S(E_2, V_2, N_2) = k \ln \Omega_2(E_2)$$

$$\Omega(E) = \int d^{3N} q d^{3N} p$$

$$E < H < E + \Delta$$

$$= \sum_{m=0}^{\frac{E}{\Delta}} \int_{E_1 < H_1 < E_1 + \Delta} d^{3N_1} q_1 d^{3N_1} p_1 \int_{E_2 < H_2 < E_2 + \Delta} d^{3N_2} q_2 d^{3N_2} p_2, E = E_1 + E_2$$

$$= \sum_{m=0}^{\frac{E}{\Delta}} \Omega_1(E_m) \times \Omega_2(E - E_m)$$

$$E_m = m\Delta$$

Notice: all terms in the sum are positive and finite.

## CAPS LOCK IS CRUISE CONTROL FOR COOL!

$\exists \bar{E}$  such that

$$\Omega_1(\bar{E})\Omega_2(E - \bar{E}) \geq \Omega_1(E_m)\Omega_2(E - E_m)$$

$$\forall m$$

$$\Omega_1(\bar{E})\Omega_2(E - \bar{E}) \leq \Omega(E) \leq \frac{E}{\Delta} \Omega_1(\bar{E})\Omega_2(E - \bar{E})$$

$$\frac{E}{\Delta} = \text{total number of terms}$$

Take Logarithm

$$S_1(\bar{E}) + S_2(E - \bar{E}) \leq S(E) \leq S_1(\bar{E}) + S_2(\bar{E}) + k \ln \left( \frac{E}{\Delta} \right)$$

Take  $N \gg 1$

1. E is extensive  $\Rightarrow E \propto N$

$\text{vol}(6N \text{ dimensional space}) \sim x^{6N}$

$$\lim_{N \rightarrow \infty} \left( \frac{\ln \frac{E}{\Delta}}{S_1(\bar{E}) + S_2(E - \bar{E})} \right) = \lim_{N \rightarrow \infty} \frac{\ln N}{6N} \neq 0$$

$$\Rightarrow S(E) = S_1(\bar{E}) + S_2(E - \bar{E})$$

AT LARGE N

1. Entropy S is extensive

2. S can be used to define temperature T

Proof: we already showed that there exists  $\bar{E}$  such that

$$S(E) = S_1(E) + S_2(E - \bar{E})$$

$$\Omega(E) = \Omega_1(\bar{E})\Omega_2(E - \bar{E})$$

$\bar{E}$  yields the maximum contribution

$$\begin{cases} d(\Omega_1(E_1)\Omega_2(E_2)) \Big|_{E_1=\bar{E}} = 0 \\ d(E_1 + E_2) = 0 \end{cases}$$

Take log

$$\begin{cases} d(\ln \Omega_1(E_1)\Omega_2(E_2)) \Big|_{E_1=\bar{E}} = 0 \\ d(E_1 + E_2) = 0 \end{cases}$$

$$d \ln(\ln \Omega_1(E_1)\Omega_2(E_2))$$

$$= dE_1 \frac{\delta \ln \Omega_1}{\delta E_1} + dE_2 \frac{\delta \ln \Omega_2}{\delta E_2}$$

$$= dE_1 \left( \frac{\delta \ln \Omega_1}{\delta E_1} - \frac{\delta \ln \Omega_2}{\delta E_2} \right)$$

Multiply by  $\kappa$

$$\frac{\delta S_1}{\delta E_1} \Big|_{E_1=\bar{E}} = \frac{\delta S_2}{\delta E_2} \Big|_{E_2=E-\bar{E}}$$

Hence define

$$\frac{1}{T} \equiv \frac{\delta S}{\delta E}$$

### 3. Equivalent definitions

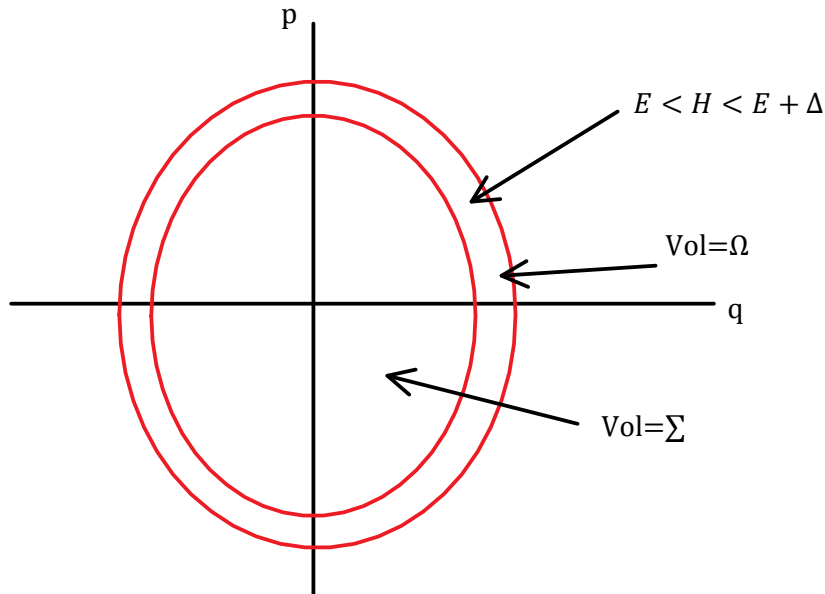
$$S(E, V, N) \equiv \kappa \ln \Sigma(E)$$

$$S(E, V, N) \equiv \kappa \ln \omega(E)$$

"equivalent" means: different, but yields same thermodynamics when we take  $N \rightarrow \infty$

$$S = \kappa \ln \Omega$$

Example



### 4. 2nd Law

"S is a non-decreasing function"

Proof

$$S = S(E, N, V)$$

But E, N fixed

Only V can change

V can only grow

$$\Sigma = \int_{H < E} d^{3N} q d^{3N} p$$

If V grows, the phase-space is growing

$\Sigma$  grows  $\Rightarrow$  S grows

### 5. 1st Law

Proof

$$S = S(E, N, V)$$

Keep N fixed and differentiate

$$dS = dE \frac{\delta S}{\delta E} + dV \frac{\delta S}{\delta V}$$

Use def of T

$$= \frac{1}{T} dE + dV \frac{\delta S}{\delta V}$$

$$\Rightarrow dE = T ds - \left( T \frac{\delta S}{\delta V} \right) dV$$

Define

$$P \equiv T \frac{\delta S}{\delta V}$$

$$\boxed{dE = T dS - P dV}$$

## Recap

Define

$$S = \kappa \ln \Omega$$

S has following properties

1. Extensive
2. Defines T (equilibrium)
3. Equivalent definitions
4. 2nd law
5. 1st law

General Prescription

1. Compute  $\Sigma$  (or  $\Omega, \omega$ )
2. Derive  $S = \kappa \ln \Sigma$   
And take  $N \rightarrow \infty$  (very large)

3. Invert relation  
 $S(E) \rightarrow E(S)$

4. Reconstruct thermodynamics

$$T = \frac{\delta U}{\delta S}$$

$$P = -\frac{\delta U}{\delta V}$$

$$F = U - TS$$

$$C_V = \frac{\delta U}{\delta T}$$

5. Derive equation of state

.....

Sphere

$$S^{D-1} \sum_{i=1}^D q_i^2 = R^2$$

$$\left\{ \begin{array}{l} \text{vol}(S^{D-1}) = \frac{2\pi^{\frac{D}{2}}}{\Gamma_E\left(\frac{D}{2}\right)} \\ \text{vol}(B^D) = \frac{\pi^{\frac{D}{2}} R^D}{\Gamma_E\left(1 + \frac{D}{2}\right)} \end{array} \right.$$

$\Gamma_E$  is euler gamma function

def

$$\Gamma_E(z) = \int_0^\infty dt t^{z-1} e^{-t}$$

properties

$$\left\{ \begin{array}{l} x\Gamma_E(x) = \Gamma_E(1+x) \\ \Gamma_E(1+m) = m! \quad m \in \mathbb{N} \\ \Gamma_E\left(\frac{1}{2}\right) = \sqrt{\pi} \end{array} \right.$$

Examples

D=2

$$\text{vol}(S') = \frac{2\pi}{\Gamma(1)} = 2\pi$$

D=3

$$\text{vol}(S') = \dots\dots\dots$$

## Ideal gas

Def

N (large!) identical, classical, free, point like particles of mass m in volume V  
Phase space

$\Gamma = \{(q_i, p_j), i, j = 1 \dots 3N, p_i, q_i \in \mathbb{R}\}$   
 Hamiltonian

$$H = \frac{1}{2m} \sum_{i=1}^{3N} p_i^2$$

Exercise: use its canonical ensemble to

1. Compute

$$\begin{aligned} \Sigma(E) &= \int_{\Gamma} d^{3N}q d^{3N}p \\ & \quad H < E \\ &= \int d^{3N}q \int_{H < E} d^{3N}p \\ &= V^N \int_{H < E} d^{3N}p \\ & \quad V \equiv \int d^{3N}q \\ & \quad H = \frac{1}{2m} \sum_i p_i^2 < E \\ & \quad \sum_{i=1}^{3N} p_i^2 < 2mE \end{aligned}$$

The integration is restricted to a 3N dimensional ball  $B^{3N}$  in momentum space  
 With a radius

$$R = \sqrt{2mE}$$

Hence

$$\boxed{\Sigma(E) = V^N \frac{\pi^{\frac{3N}{2}} R^{3N}}{\Gamma\left(1 + \frac{3}{2}N\right)}}$$

$$= \frac{(2\pi m E V^{\frac{2}{3}})^{\frac{3N}{2}}}{\left(\frac{3N}{2}\right)!}$$

(N even!)

2.  $S = \kappa \ln \Sigma$

$$= \kappa \ln \frac{(2\pi m E V^{\frac{2}{3}})^{\frac{3N}{2}}}{\left(\frac{3N}{2}\right)!}$$

Take  $N \rightarrow$  large

Stirling approximation

$$\ln m! \approx m \ln m - m$$

$$= \frac{3}{2} N \kappa \ln \left( \frac{(2\pi m E V^{\frac{2}{3}})^{\frac{3}{2}}}{\frac{3}{2} N \kappa \ln \frac{3}{2} N + \frac{3}{2} N \kappa} \right)$$

$$= \ln e$$

$$= \frac{3}{2} N \kappa \ln \left[ \frac{3\pi e}{3} m e = E V^{\frac{2}{3}} \right]$$

Define

$$\mu_0 \equiv \frac{4\pi e}{3} M$$

$$\boxed{S = \frac{3}{2} N \kappa \ln \left( \frac{\mu_0 E V^{\frac{2}{3}}}{N} \right)}$$

3. Invert  $S(E) \rightarrow E(S)$

$$\frac{2S}{3N\kappa} = \ln \left( \frac{\mu_0 E V^{\frac{2}{3}}}{N} \right)$$

$$\exp\left[\frac{2S}{3N\kappa}\right] = \frac{\mu_0 E V^{\frac{2}{3}}}{N}$$

$$E = \frac{N}{\mu_0 V^{\frac{2}{3}}} \exp\left[\frac{2S}{3N\kappa}\right]$$

#### 4. Thermodynamics

$$T = \frac{\delta E}{\delta S}$$

Maxwell relation

$$= \frac{2}{3N\kappa} E \Rightarrow E = \frac{3}{2} N\kappa T$$

$$\Rightarrow C_V = \frac{\delta E}{\delta T} = \frac{3}{2} N\kappa$$

$$P = -\frac{\delta E}{\delta V}$$

Maxwell relation

$$= -\left(-\frac{3}{2}\right) \frac{1}{V} E = \frac{2E}{3V}$$

$$= \frac{2}{3V} \left(\frac{3}{2} N\kappa T\right)$$

$$P = \frac{N\kappa T}{V}$$

#### 2. Gibbs paradox

Ideal gas (example)

$$S = \frac{3}{2} Nk \ln \frac{\mu_0' E v^{\frac{2}{3}}}{N}$$

From explicit calculation

$$E = \frac{3}{2} NkT$$

$$S = \frac{3}{2} Nk \ln cTV^{\frac{2}{3}}$$

Compute difference in entropy

$$\Delta S = S - S_1 - S_2$$

$$= \frac{3}{2} Nk \ln(cTV^{\frac{2}{3}}) - \frac{3}{2} N_1 k \ln(cTV_1^{\frac{2}{3}}) - \frac{3}{2} N_2 k \ln(cTV_2^{\frac{2}{3}})$$

$$\Delta S = k \left( N_1 \ln \frac{V}{V_1} + N_2 \ln \frac{V}{V_2} \right)$$

$$V > U_1, U_2$$

$$\Rightarrow \Delta S > 0$$

Compare to

$$1 \text{ blue} \quad 2 \text{ yellow}$$

Same T,P, suppose the 2 gasses have different "colour"

$$\boxed{\quad | \quad}$$

Solution to the paradox

New rule:

Any time there are N indistinguishable particles, add a factor of 1/N!

$$\Sigma(E) = \frac{1}{p^{3N} N!} \int_{H < E} d^{3N} q d^{3N} p$$

$$S_{new} = S_{old} - k \ln N!$$

$$N \gg 1$$

$$= S_{old} - kN \ln N$$

$$= \frac{3}{2} Nk \ln c T V^{\frac{2}{3}} - kN \ln N$$

$$S = \frac{3}{2} Nk \ln C T \left(\frac{V}{N}\right)^{\frac{2}{3}}$$

$$\Delta S = k(N \ln \left(\frac{V}{N}\right)^{\frac{2}{3}} - N_1 \ln \left(\frac{V_1}{N_1}\right)^{\frac{2}{3}} - N_2 \ln \left(\frac{V_2}{N_2}\right)^{\frac{2}{3}})$$

$$= 0$$

$$\text{Because } \frac{V}{N} = \frac{V_1}{N_1} = \frac{V_2}{N_2}$$

In the case of different gases

$$\Sigma = \frac{1}{p^{3N} N_1! N_2!} \int_{H < E} d^{3N} q d^{3N} p$$

$$\frac{1}{N!} \neq \frac{1}{N_1! N_2!} \Rightarrow \Delta S > 0$$

Still true for different gases

3. Third Law?

$$S = \frac{3}{2} Nk \ln C T \left(\frac{V}{N}\right)^{\frac{2}{3}}$$

When  $T \rightarrow 0$  problem

Keep c, V, N constant

$$\lim_{T \rightarrow 0} S \rightarrow -\infty$$

Exercise: paramagnet

1. N particles

2. E energy (fixed)

$$3. \Gamma = \{\{\sigma_i\}, \sigma_i = \pm 1\}$$

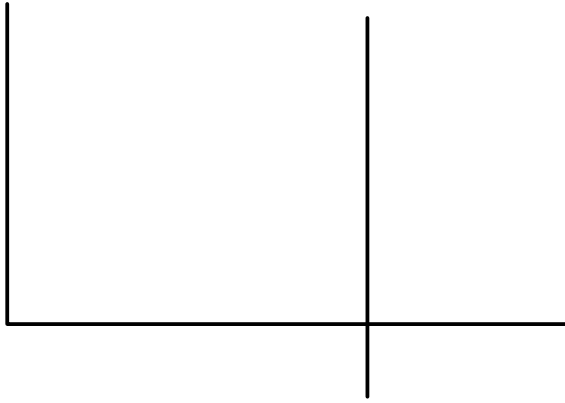
$$4. H = -\mu h_M \sum_{i=1}^N \sigma_i$$

$h_M \Rightarrow$  magnetic field

Compute entropy







Exercise: 2 state system (model of paramagnet)

Using microcanonical ensemble (in qm)

Microscopic description

1. N particles (fixed)
2. E energy (fixed)
3.  $\Gamma = \{\{\sigma_i\}_i^N, \sigma_i = \pm 1\}$   
Ie requires ?
4.  $H = -\mu p_m \sum_{i=1}^N \sigma_i$   
?????

No kinetic or potential term in H

Macroscopic description

- $N_+$   
# occurrences of '+'
- $N_-$   
# occurrences of '-'

This is a QM system!

Discrete set of states

$$\Omega \equiv \frac{1}{h^{3N}} \int_{H < E} d^{3N}q d^{3N}p \xrightarrow{\text{REPLACE}} \Omega: \# \text{ microstates } (\{+ \dots \pm\})$$

Satisfying macroscopic constraints counting!

Two constraints: E, N fixed

$$\begin{cases} E = -\mu P_m (N_+ - N_-) \\ N = N_+ + N_- \end{cases}$$

$$\epsilon \equiv \frac{E}{\mu P_m N}$$

$$N_{\pm} \equiv \frac{N}{2} (1 \mp \epsilon)$$

$$-1 \leq \epsilon \leq +1$$

$$\Omega = \binom{N}{N_+}$$

$$= \frac{N!}{N_+! (N - N_+)!} = \frac{N!}{N_+! N_-!}$$

$N_+$  and  $N_-$

known. You want to know how many different sequences  $\{+ - + + \dots +\}$  contain exactly

- $N_+$  +  
 $N_-$  -

Start with one such sequence

{+, +, ..., +, -, -, -, ..., -}

All others obtained by changing order

⇒ factor of  $N!$

BUT: overcounting! Exchanging identical symbols yields same sequence

$$\Rightarrow \text{factors of } \frac{1}{N_+! N_-!} \Rightarrow \Omega = \frac{N!}{N_+! N_-!}$$

$$S = k \ln \Omega$$

$$= k \ln \frac{N!}{N_+! N_-!}$$

Stirling approximation

$$\ln N! \sim N \ln N - N$$

$$= k(N \ln N - N - N_+ \ln N_+ + N_+ - N_- \ln N_- + N_-)$$

$$= k(N \ln N - N_+ \ln N_+ - N_- \ln N_-)$$

$$= k \left( N \log N - \frac{N}{2} (1 - \epsilon) \ln \left[ \frac{N}{2} (1 - \epsilon) \right] - \frac{N}{2} (1 + \epsilon) \ln \left[ \frac{N}{2} (1 + \epsilon) \right] \right)$$

$$= k \left\{ N \ln N - \frac{N}{2} (1 + \epsilon) \ln N - \frac{N}{2} (1 + \epsilon) \ln \frac{(1 - \epsilon)}{2} - \frac{N}{2} (1 + \epsilon) \ln N - \frac{N}{2} (1 + \epsilon) \ln \frac{(1 + \epsilon)}{2} \right\}$$

$$= k \left\{ -\frac{N}{2} (1 + \epsilon) \ln \frac{(1 - \epsilon)}{2} - \frac{N}{2} (1 + \epsilon) \ln \frac{(1 + \epsilon)}{2} \right\}$$

$$= \boxed{-\frac{kN}{2} \ln \left[ \left( \frac{1 - \epsilon}{1} \right)^{1 - \epsilon} \left( \frac{1 + \epsilon}{2} \right)^{1 + \epsilon} \right]} = S$$

Compute T

$$\frac{1}{T} = \frac{\delta S}{\delta E}$$

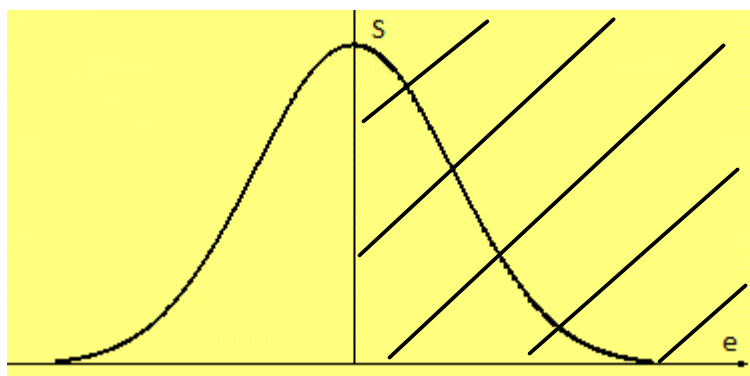
$$= \left( \frac{\delta E}{\delta \epsilon} \right)^{-1} \frac{\delta S}{\delta \epsilon}$$

$$= \frac{1}{\mu P_m N} \times \frac{\delta}{\delta \epsilon} \left[ -\frac{Nk}{2} \left( (1 - \epsilon) \ln(1 - \epsilon) + (1 + \epsilon) \ln(1 + \epsilon) - 2 \ln 2 \right) \right]$$

$$= -\frac{k}{2\mu P_m} (-P(1 - \epsilon) - 1 + P_m(1_\epsilon) + 1)$$

$$\Rightarrow \boxed{\frac{1}{T} = \frac{k}{2\mu P_m} \ln \left( \frac{1 - \epsilon}{1 + \epsilon} \right)}$$

Plot  $T(\epsilon), S(\epsilon)$



1.  $\epsilon > 0 \Rightarrow$  problem,  $T < 0$  imphyiscal (though maths correct)

We did not take into account the possibility that particles MOVE

H should contain kinetic and potential terms

$\epsilon$  MUST be negative

2. With this Caviat fixed

$S(T)$  becomes monotonic

3. Third law of thermodynamics is reproduced

When

$$\epsilon \rightarrow -1$$

$$N_+ \rightarrow N$$

There is only 1 state

$$\{+, +, \dots, +, +\}$$

$$\ln 1 = 0$$

This is useful because quantized(=discrete) states

Classical system

Phase-space:

$$\Gamma = \left\{ \{P_{mk}, q_{mj}\}, m = 1, \dots, N, k, j = 1, 2, 3 \right\}$$

$P_{mk}$  3N matrix

$q_{mj}$  3N coordinates

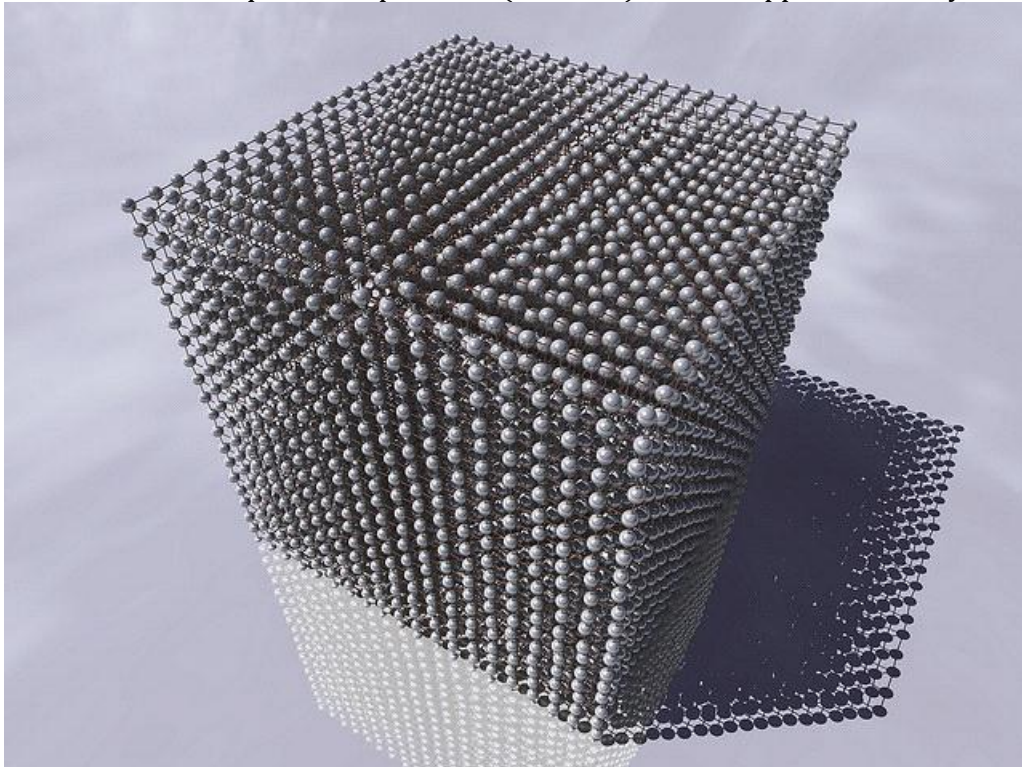
$$H = \sum_{i=1}^N H_i$$

$$H_i = \frac{1}{2m} \sum_{k=1}^3 P_{ik}^2 + \frac{1}{2} m \omega^2 \sum_{k=1}^3 q_{ik}^2$$

3N harmonic oscillators

Approximate model of a solid:

Osc around equilibrium positions (if SMALL) are well approximated by harmonic oscillator



$$\Sigma(E) = \frac{1}{h^{3N}} \int_{H < E} d^{3N}q d^{3N}p$$

1. No  $1/N!$  because particles can be distinguished by their "lattice" position

2. You could compute  $\Omega(E)$

$$\Sigma(E) = \frac{1}{h^{3N}} \int_{H < E} d^{3N}q d^{3N}p$$

$$\frac{1}{2m} \sum_{i=1}^3 P_i^2 + \frac{1}{2} m \omega^2 \sum_{i=1}^3 q_i^2$$

Do a change of variable in the integration!

Define  $6N$  variables  $x_i$

$$x_i = \begin{cases} \frac{1}{\sqrt{2m}} p_i & \text{when } i = 1, \dots, 3N \\ \sqrt{\frac{m\omega^2}{2}} q_{i-3N} & \text{when } i = 3N + 1, \dots, 6N \end{cases}$$

A point in  $\Gamma$  is  $\{p_1, p_2, p_3, \dots, q_1, q_2, q_3, \dots\}$

$$p_1, p_2, p_3, \dots = x_1, \dots, x_{3N}$$

$$q_1, q_2, q_3, \dots = x_{3N+1}, \dots, x_{6N}$$

The constraint reads

$$\sum_{i=1}^{6N} x_i^2 \leq E$$

$6N$  dimensional ball with radius  $R = \sqrt{E}$

$$\Sigma(E) = \frac{1}{h^{3N}} \int_{H < E} d^{3N} q d^{3N} p$$

$$= \frac{1}{h^{3N}} \int_{\Sigma x^2 \leq E} d^{6N} x (\sqrt{2m})^{3N} \left( \sqrt{\frac{2}{m\omega^2}} \right)^{3N}$$

$$(\sqrt{2m})^{3N} \left( \sqrt{\frac{2}{m\omega^2}} \right)^{3N} = \text{jacobian}$$

$$dp_i = dx_i \sqrt{2m}$$

$$= \left( \frac{2}{h\omega} \right)^{3N} \text{vol}(B^{6N}(R = \sqrt{E}))$$

$$= \left( \frac{2}{h\omega} \right)^{3N} * \frac{\pi^{\frac{6N}{2}} R^{6N}}{\Gamma_E \left( 1 + \frac{6N}{2} \right)}$$

$$= \left( \frac{2\pi E}{h\omega} \right)^{3N} * \frac{1}{(3N)!}$$

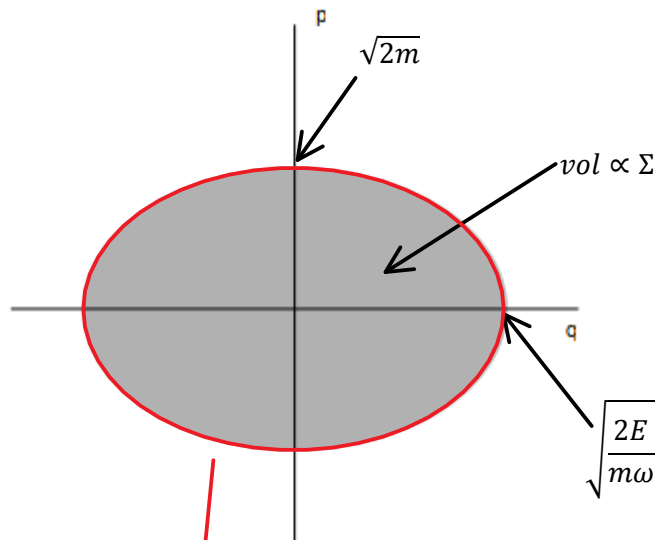
$6N \rightarrow 2$

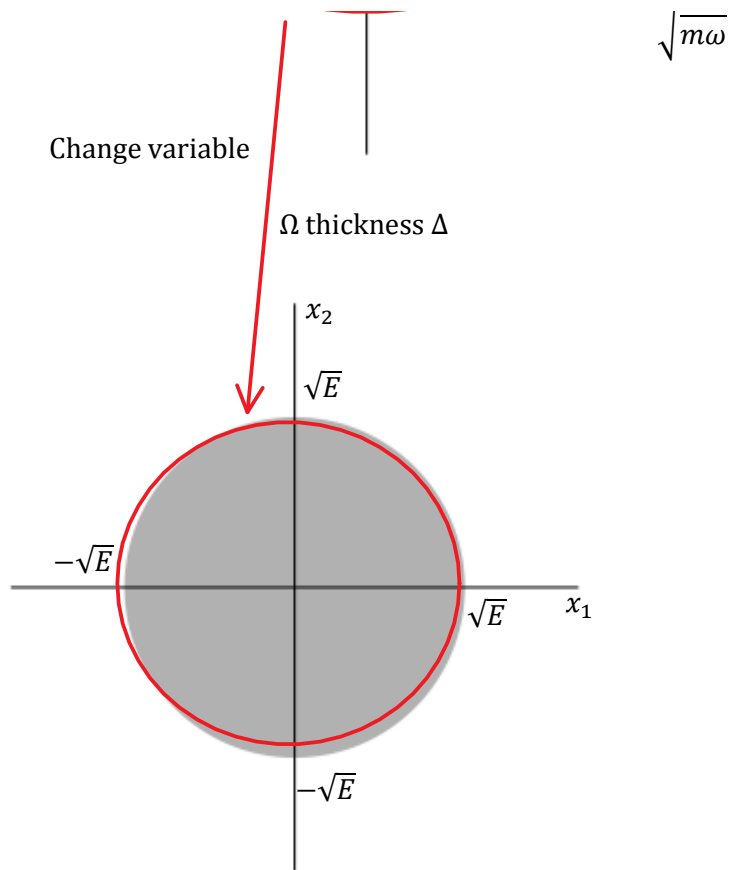
(i.e. suppose you have only one harmonic oscillator)

$$\Gamma = \left\{ \begin{matrix} \{q\} \\ \{p\} \end{matrix} \right\}$$

$$H = \frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 q^2 \leq E$$

Ellipse





$$x_{6N} = \sqrt{\frac{m\omega^2}{2}} q_{3N}$$

$$dx_{6N} = \sqrt{\frac{m\omega^2}{2}} dq_{3N}$$

$$dq_{3N} = \sqrt{\frac{2}{m\omega^2}} dx_{6N}$$

$$dp_{3N} = \sqrt{2m} dx_{6N}?$$

$$\Sigma = \left(\frac{2\pi E}{h\omega}\right)^{3N} * \frac{1}{(3N)!}$$

Compute S (for large N)

Write all equations/definitions beforehand- helpful

$$S \equiv k \ln \Sigma(E)$$

$$= k \ln \left[ \left(\frac{2\pi E}{h\omega}\right)^{3N} * \frac{1}{(3N)!} \right]$$

Stirling

$$\ln 3N! \sim 3N \ln 3N - 3N$$

$$= 3Nk \ln \left(\frac{2\pi E}{h\omega}\right) - k(3N \ln 3N - 3N)$$

$$= 3Nk \left[ 1 + \ln \left(\frac{2\pi E}{h\omega}\right) \right] = S$$

$$E = \frac{3N\hbar\omega}{2\pi e} \exp \left[ \frac{S}{3Nk} \right]$$

$$T = \frac{\delta E}{\delta S} = \frac{E}{3Nk} \Rightarrow \boxed{E = 2NkT}$$

$$C_v = \frac{\delta E}{\delta T} = 3Nk$$

Equipartitions in H there are  
 $3N q_i$ , and  $3N p_i$

Entering quadratically

$$C_V = (3N + 3N) \frac{1}{2} k = 3Nk$$

In S, replace  $E=3NkT$

$$S = 3Nk \left( 1 + \ln \left( \frac{kT}{\hbar\omega} \right) \right)$$

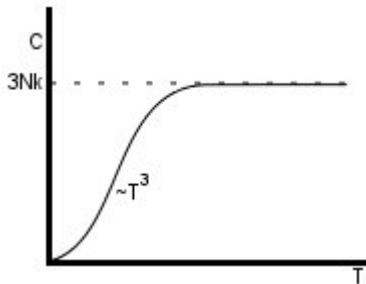
$$\hbar = \frac{h}{2\pi}$$

#### 4. Violations of equipartition theorem

Example: Solid

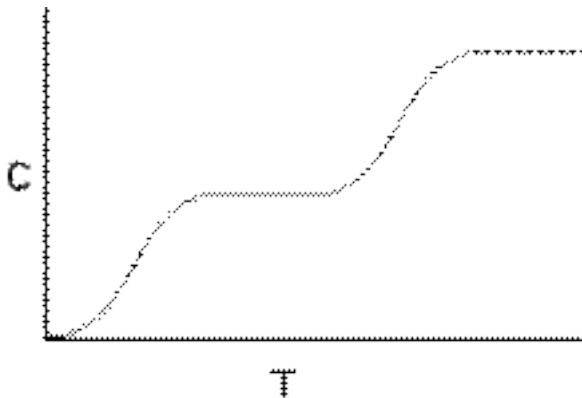
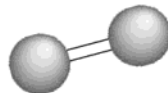
$$C_v = 3NK$$

Dulong-petit law



Solution involves QM

Example 2: Diatomic gas



No classical explanation (QM needed)

One can at best produce classical models that work well over ranges of  $T$

$$1) H = \frac{1}{2M} \sum_i P_i^2$$

$P$ : c. m. momentum

2) Rotation D. O. F.

$$H = \frac{1}{2M} \sum_i P_i^2 + \frac{1}{2I} \sum_i e_i^2$$

I: momentum of inertia

e: angular momentum

Equipartition

$$C_V = N \times \frac{k}{2} \times (3 + 2)$$

$$= \frac{5}{2} Nk$$

$$3) H = \frac{1}{2M} \sum_i P_i^2 + \frac{1}{2I} \sum_i e_i^2 + \frac{1}{2\mu} \sum_i p_i^2 + \frac{1}{2} \mu \omega^2 \sum_i (R_i - R_0)^2$$

$\mu$ : reduced mass

$R_i$ : distance between atoms

( $R_0$  average)

$p_i$ : momentum conjugate to  $R_i$

Equipartition

$$C_V = \frac{1}{2} Nk(3 + 2 + 1 + 1)$$

$$= \frac{7}{2} Nk$$

Concept of energy threshold (QM) in order to connect 1-2-3

Microcanonical ensemble (classical)

Good

- 1) 1st, 2nd law
- 2) EQ state computed
- 3) At ordinary T, Equipartition theorem works

Bad

- 1) What is h?
- 2)  $\frac{1}{N!}$  boltzmann factor?
- 3) Third law?
- 4) Exp. Violations of equipartition

Ugly

- 1) Calculations are hard!
- 2) N, E fixed Unphysical!

### CANONICAL ENSEMBLE

Addresses 2) ugly feature and makes calculations more accessible!

### Partition Function

Classical canonical ensemble

Assumptions

1. Physical systems of interest are in contact (equilibrium) with a heat reservoir at temperature T
2. N fixed

### NO REFERENCE TO E

Density function

$$\rho = (q, p) \equiv e^{-\frac{1}{kT} H(q, p)}$$

$$= e^{-\beta H(p, q)}$$

$$\beta = \frac{1}{kT}$$

Partition function

$$Z_N = \frac{1}{h^{3N} N!} \int_{\Gamma} d^{3N} q d^{3N} p e^{-\beta H}$$

$\Gamma \leftarrow$  integral over whole phase-space

$$\frac{1}{h^{3N} N!} = \text{same as microcanonical}$$

Define Helmholtz free energy as

$$Z_N \equiv e^{-\beta F(v,T)}$$

Show that

1. F is extensive
2. F satisfies  $F = U - TS$

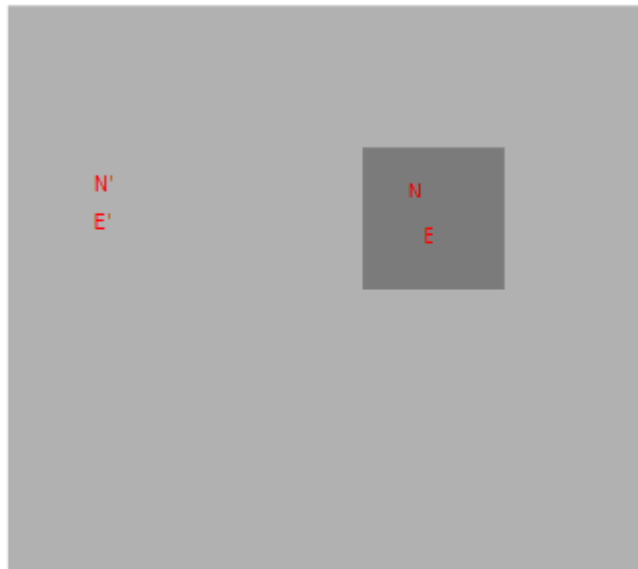
Derivation:

System N,E

Reservoir N', E'

$E' \gg E$

$N' \gg N$



$$E_T = E + E'$$

$$N_T = N + N'$$

USE Microcanonical

$$\Omega(E_T) = \int_{E_T < H < E_T + 2\Delta} d^{3N} q d^{3N} p d^{3N} q' d^{3N} p'$$

Assume particles distinguishable and  $h=1$

$d^{3N} q d^{3N} p =$  coordinates and momentua of system

$d^{3N} q' d^{3N} p' =$  of resevoir

$$= \sum_E \int_{E < H < E + \Delta} d^{3N} q d^{3N} p \int_{E' < H < E' + \Delta} d^{3N} q' d^{3N} p'$$

$$= \sum_E \int_{E < H < E + \Delta} d^{3N} q d^{3N} p \Omega'(E')$$

$$= \sum_E \int_{E < H < E + \Delta} d^{3N} q d^{3N} p \Omega'(E_T - H)$$

We know that

$$S'(E_T - H) = k \ln \Omega'(E_T - H)$$

Taylor expand

$$= k \ln \Omega'(E_T) - k \frac{\delta \ln \Omega'(E_T)}{\delta E_T} H + \dots$$

$$\cong S'(E_T) - \frac{\delta S'}{\delta E_T} H$$

$$= S'(E_T) - \frac{1}{T} H$$

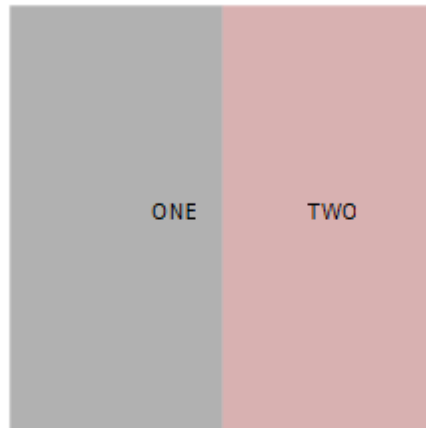
$$\Omega'(E_T - H) = \exp \left[ \frac{1}{k} S' \right]$$



$$\begin{aligned}
&= \exp\left[\frac{S(E_T)}{k}\right] \exp\left[-\frac{H}{kT}\right] \\
\Omega(E_T) &= \exp\left[\frac{S(E_T)}{k}\right] \sum_E \int_{E < H < E + \Delta} d^{3N}q d^{3N}p e^{-\frac{H}{kT}} \\
&= \exp\left[\frac{S(E_T)}{k}\right] \int_{\Gamma} d^{3N}q d^{3N}p e^{-\frac{H}{kT}} \\
\exp\left[\frac{S(E_T)}{k}\right] &= \text{constand that is not interesting for our system}
\end{aligned}$$

Essentive:

Proof:



Take  $h=1$

$$N = N_1 + N_2$$

Same temperature T

$$Z_N = \frac{1}{N_1!} \frac{1}{N_2!} \int d^{3N}q d^{3N}p e^{-\beta H}$$

$$H = H_1 + H_2$$

As long as the interactions are short ranged,  $H=H_1+H_2$

$$\begin{aligned}
&= \frac{1}{N_1! N_2!} \int d^{3N}q_1 d^{3N}p_1 d^{3N}q_2 d^{3N}p_2 e^{-\beta H_1} e^{-\beta H_2} \\
&= \left[ \frac{1}{N_1!} \int d^{3N}q_1 d^{3N}p_1 e^{-\beta H_1} \right] \times \left[ \frac{1}{N_2!} \int d^{3N}q_2 d^{3N}p_2 e^{-\beta H_2} \right] \\
&= Z_{N_1} Z_{N_2} \\
F &= -kT \ln Z_N \\
&= -kT \ln Z_{N_1} Z_{N_2} \\
&= -kT \ln Z_{N_1} - kT \ln Z_{N_2} \\
&= F_1 + F_2
\end{aligned}$$

Prove that  $F = U - TS$

We defined

$$e^{-\beta f} \equiv \frac{1}{h^{3N} N!} \int d^{3N}q d^{3N}p e^{-\beta H}$$

Rewrite as

$$1 = \frac{1}{h^{3N} N!} \int d^{3N}q d^{3N}p e^{-\beta(H-F)}$$

Take derivative in respect to  $\beta$

$$0 = \frac{1}{h^{3N}N!} \int d^{3N}q d^{3N}p e^{-\beta(H-F)} \frac{\delta}{\delta\beta} (-\beta(H-F))$$

$$= \frac{1}{h^{3N}N!} \int d^{3N}q d^{3N}p e^{-\beta(H-F)} \times \left[ F - H + \beta \frac{\delta F}{\delta\beta} \right]$$

Internal energy can (must) be defined be ensemble average

$$E = U = \langle H \rangle$$

$$= \int \frac{d^{3N}q d^{3N}p}{h^{3N}N!} e^{-\beta(H-F)} H$$

Remember

$$\langle p \rangle = \frac{\int d \dots p \times f}{\int d \dots \rho}$$

Rewrite

$$0 = \left( F + \beta \frac{\delta F}{\delta\beta} \right) \times \frac{1}{h^{3N}N!} \int d^{3N}q d^{3N}p e^{-\beta(H-F)} - \frac{1}{h^{3N}N!} \int d^{3N}q d^{3N}p e^{-\beta(H-F)}$$

$$= \left( F + \beta \frac{\delta F}{\delta\beta} \right) \times \frac{1}{h^{3N}N!} \int d^{3N}q d^{3N}p e^{-\beta(H-F)} - U$$

$$0 = F - U + \beta \frac{\delta F}{\delta\beta}$$

$$\beta = \frac{1}{kT}$$

$$\beta \frac{\delta F}{\delta\beta} = \beta \left( \frac{\delta\beta}{\delta T} \right)^{-1} \frac{\delta}{\delta T} F$$

$$= \frac{1}{kT} \left( -\frac{1}{kT^2} \right)^{-1} \frac{\delta F}{\delta T}$$

$$= -T \frac{\delta F}{\delta T}$$

$$0 = F - U - T \frac{\delta F}{\delta T}$$

Maxwell

$$S = -\frac{\delta F}{\delta T}$$

$$\Rightarrow \boxed{F = U - TS}$$

# Canonical ensemble

23 November 2011

09:10

## Prescription

1. Compute

$$Z_N = \frac{1}{h^{3N} N!} \int_{\Gamma} d^{3N} q d^{3N} p e^{-\beta H}$$

$N!$  = indistinguishable particles

$$\beta = \frac{1}{kT}$$

2. Compute Free energy

$$F = -kT \ln Z_N$$

3. Maxwell relations

$$S = -\frac{\delta F}{\delta T}$$

$$P = -\frac{\delta F}{\delta V}$$

4. Thermodynamics

## Exercise N.1: monoatomic ideal gas

$$H = \frac{1}{2m} \sum_{i=1}^{3N} p_i^2$$

$N$  particles

$V$  volume

$$\int_{-\infty}^{\infty} dx e^{-\gamma x^2} = \sqrt{\frac{\pi}{\gamma}}$$

Set  $h=1$  for simplicity

$$Z_N = \frac{1}{N!} \int_{\Gamma} d^{3N} q d^{3N} p e^{-\beta H}$$

$$\begin{aligned} &= \frac{1}{N!} \int_{\Gamma} dq_1 dq_2 \dots dq_{3N} dp_1 dp_2 \dots dp_{3N} e^{-\frac{\beta}{2m} \sum_i p_i^2} \\ &= \frac{1}{N!} * V^N * \int_{-\infty}^{\infty} dp_1 e^{-\frac{\beta}{2m} p_1^2} * \int_{-\infty}^{\infty} dp_2 e^{-\frac{\beta}{2m} p_2^2} * \int_{-\infty}^{\infty} dp_3 e^{-\frac{\beta}{2m} p_3^2} \\ &= \frac{V^N}{N!} \left[ \int_{-\infty}^{\infty} dp e^{-\frac{1}{2mkT} p^2} \right]^{3N} = \frac{V^N}{N!} (\sqrt{2\pi mkT})^{3N} \\ &= \frac{V^N T^{\frac{3N}{2}} C^{\frac{3N}{2}}}{N!} \end{aligned}$$

$C$ =arbitrary constant

$$F = -kT \ln Z_N$$

$$= -kT \ln \frac{V^N (cT)^{\frac{3}{2}N}}{N!}$$

$$= -NkT \ln \left[ \frac{V}{N} cT^{\frac{3}{2}} \right]$$

$$P = -\frac{\delta F}{\delta V} = -(-NkT) \frac{1}{V} = \frac{NkT}{V} \Rightarrow \boxed{PV = NkT}$$

$$S = -\frac{\delta F}{\delta T} = Nk \ln \left( \frac{V}{N} cT^{\frac{3}{2}} \right) + NkT \left( \frac{3}{2T} \right)$$

$$\begin{aligned}
&= \frac{F}{T} + \frac{3}{2} Nk \\
E = U &= F + TS \\
&= F + T \left( -\frac{F}{T} + \frac{3}{2} Nk \right) \\
&= F - F + \frac{3}{2} NkT \Rightarrow \boxed{U = \frac{3}{2} NkT} \Rightarrow \boxed{C_v = \frac{\delta U}{\delta T} = \frac{3}{2} Nk}
\end{aligned}$$

1. As long as N large, Microcanonical and canonical ensembles yield same thermodynamics
2. Be precise at early stages

Exercise N.2 Diatomic ideal gas  
(Room T)

$$H = \sum_i \frac{1}{2m} p_i^2 + \frac{1}{2I} l_i^2$$

Where phase-space is

$$\Gamma = \{ \{ \bar{Q}_i, \bar{P}_i, \theta_i, \phi_i, \bar{l}_i \}, i = 1 \dots N \}$$

$\theta_i, \phi_i \rightarrow (h = 1)$  describing rotation, not  $d\theta d\phi$

$\bar{l}_i$  only two ways of rotation

???

$$\begin{aligned}
Z_N &= \frac{1}{N!} \int d^{3N} Q d^{3N} P d^N \cos \theta d^N \phi d^{2N} l e^{-\beta H} \\
&= \frac{1}{N!} V^N (4\pi)^N
\end{aligned}$$

$4\pi = \text{angles}$

Why 2N

N particles  $\bar{l}$  vector  $\begin{pmatrix} l_1 \\ l_2 \\ l_3 \end{pmatrix}$

But diatomic: 2 meaningful components, so 2N

$$\begin{aligned}
Z_N &= V^N (4\pi)^N \int dP_1 dP_2 \dots dP_{3N} dl_1 dl_2 \dots dl_{2N} \exp -\beta \left[ \sum_i \frac{1}{2m} p_i^2 + \sum_i \frac{1}{2I} l_i^2 \right] \\
&= \frac{1}{N!} V^N (4\pi)^N \left[ \int dP e^{-\frac{1}{2mkT} P^2} \right]^{3N} \left[ \int dl e^{-\frac{1}{IkT} l^2} \right]^{2N} \\
&= \frac{1}{N!} v^N (4\pi)^N (2\pi mkT)^{\frac{3N}{2}} (2\pi IkT)^{\frac{3N}{2}}
\end{aligned}$$

$$Z_N = \frac{V^N (cT)^{\frac{5N}{2}}}{N!}$$

$$F = -kT \ln Z_N$$

$$= -kT \ln \left( \frac{V^N (cT)^{\frac{5N}{2}}}{N!} \right)$$

$$\ln N! \approx N \ln N - N$$

$$= -NkT \ln \left( \frac{V^N (cT)^{\frac{5}{2}}}{N} \right) - N \cong -NkT \ln \left( \frac{V^N (cT)^{\frac{5}{2}}}{N} \right)$$

$$P = -\frac{\delta F}{\delta V} = \frac{NkT}{V} \Rightarrow \boxed{PV = NkT}$$

$$S = -\frac{\delta F}{\delta T} = -\frac{F}{T} + NkT \left( \frac{5}{2} \frac{1}{T} \right)$$

$$\boxed{C_v = \frac{5}{2} Nk}$$

# QM Canonical ensemble

24 November 2011

09:07

Pragmatic approach

Classical

Phase-space  $\Gamma$

QM

- Discrete energy levels

$\hat{\epsilon}_k$ , occupation number  $\hat{m}_k$

Sequence of  $\{\hat{m}_k\}$  replaces  $\Gamma$

- $E = \sum_k \hat{m}_k \hat{\epsilon}_k$

Sum of levels

- $\Omega(\epsilon) = \int_{\Gamma(E < H < E + \Delta)} d^{3N}q d^{3N}p \leftrightarrow \Omega(\epsilon) = \sum_{\{\hat{m}_k\}} W(\{\hat{m}_k\})$

$W$ : number of different ways to realize/write same state

Example: 2 state system

$N_+, N_-$

$$W = \binom{N}{N_+}$$

Harmonic oscillator (QM)

$$H = \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 Q^2$$

Eigenstates

$$\hat{\epsilon}_k = \left(k + \frac{1}{2}\right) \hbar \omega$$

$$k \in N_0$$

(no degeneracies)

Exercise: compute canonical ensemble for system of 3N oscillators which are decoupled and have all same  $\omega$

(Einstein solid)

Compute partition function

$$Z_N = \sum_{m_1=0}^{\infty} \exp(-\beta \hat{\epsilon}_{m_1}) * \sum_{m_2=0}^{\infty} \exp(-\beta \hat{\epsilon}_{m_2}) * \dots * \sum_{m_{3N}=0}^{\infty} \exp(-\beta \hat{\epsilon}_{m_{3N}})$$

Because  $\omega$  is same, AND decoupled oscillators

$$= \left[ \sum_{(m=0)}^{\infty} \exp\left(-\beta \left(m + \frac{1}{2}\right) \hbar \omega\right) \right]^{3N}$$

Because no degeneracies, summation can be done explicitly

$$= \left[ \exp\left(-\frac{\beta \hbar \omega}{2}\right) \right]^{3N} \left[ \sum_{m=0}^{\infty} \exp(-\beta m \hbar \omega) \right]^{3N}$$

$$= \left[ \exp\left(-\frac{\beta \hbar \omega}{2}\right) \right]^{3N} [1 + \exp(-\beta \hbar \omega) + (\exp(-\beta \hbar \omega))^2 + \dots]^{3N}$$

$\beta \hbar \omega > 0 \Rightarrow \exp(-\beta \hbar \omega) < 1$

Geometric series

$$= \left[ \exp\left(-\frac{\beta \hbar \omega}{2}\right) \right]^{3N} \left[ \frac{1}{1 - \exp[-\beta \hbar \omega]} \right]^{3N}$$

$$= \left[ \frac{\exp\left(-\frac{\beta \hbar \omega}{2}\right)}{\exp\left(-\frac{\beta \hbar \omega}{2}\right) (\exp\left(\frac{\beta \hbar \omega}{2}\right) - \exp\left(-\frac{\beta \hbar \omega}{2}\right))} \right]^{3N}$$

$$= \left[ \frac{1}{(\exp\left(\frac{\beta \hbar \omega}{2}\right) - \exp\left(-\frac{\beta \hbar \omega}{2}\right))} \right]^{3N}$$

$$= \left[ \frac{1}{2 \sinh\left(\frac{\beta \hbar \omega}{2}\right)} \right]^{3N} = Z_N$$

Free energy

$$F = -kT \ln Z_N$$

$$= 3NkT \ln \left[ 2 \sinh\left(\frac{\beta \hbar \omega}{2}\right) \right]$$

$$S = -\frac{\delta F}{\delta T}$$

$$= -\frac{\delta}{\delta T} \left( 3NkT \ln \left[ 2 \sinh\left(\frac{\hbar \omega}{2kT}\right) \right] \right)$$

$$= -3Nk \ln \left[ 2 \sinh\left(\frac{\hbar \omega}{2kT}\right) \right] - 3NkT \frac{1}{2 \sinh\left(\frac{\hbar \omega}{2kT}\right)} 2 \cosh\left(\frac{\hbar \omega}{2kT}\right) * \left(-\frac{\hbar \omega}{kT^2}\right)$$

$$= -3Nk \ln \left[ 2 \sinh\left(\frac{\hbar \omega}{2kT}\right) \right] + \frac{3N\hbar \omega}{2T} \coth\left(\frac{\hbar \omega}{2kT}\right)$$

$$S_{classical} = 3Nk \left[ 1 + \ln \frac{kT}{\hbar \omega} \right]$$

From classical calculation

Take several limits and compare

$$T \rightarrow \infty \quad x = \frac{\hbar \omega}{2kT} \rightarrow 0$$

$$\coth x \sim \frac{1}{x} \quad \text{for } x \rightarrow 0$$

$$\sinh x \sim x \quad \text{for } x \rightarrow 0$$

$$S_{QM} \approx_{large T} -3Nk \ln \frac{\hbar \omega}{kT} + \frac{3N\hbar \omega}{2T} \frac{2kT}{\hbar \omega}$$

$$= -3Nk \ln \frac{\hbar \omega}{kT} + \frac{3Nk}{T}$$

$$= -3Nk \left[ \ln \frac{kT}{\hbar \omega} + 1 \right]$$

What about  $T \rightarrow 0$

Then  $x \rightarrow \infty$

$$\text{And } \begin{cases} \coth x \rightarrow 1 \\ \sinh x \rightarrow \frac{e^x}{2} \end{cases}$$

$$S_{QM} \approx_{small T} -3Nk \ln \left[ 2 * \frac{\exp\left[\frac{\hbar \omega}{2kT}\right]}{2} \right] + \frac{3N\hbar \omega}{2T} * 1$$

$$= -3Nk \frac{\hbar \omega}{2kT} + \frac{3N\hbar \omega}{2T}$$

$$= -\frac{3N\hbar \omega}{2T} + \frac{3N\hbar \omega}{2T} = 0$$

THIRD LAW!

Internal energy

$$S = -\frac{F}{T} + \frac{3N\hbar\omega}{2t} \coth \frac{\hbar\omega}{2kT}$$

Compute

$$\begin{aligned} U = E = F + TS \\ &= F + T \left( -\frac{F}{T} + \frac{3N\hbar\omega}{2t} \coth \frac{\hbar\omega}{2kT} \right) \\ &= \frac{3}{2} N\hbar\omega \coth \left( \frac{\hbar\omega}{2kT} \right) \end{aligned}$$

For  $T \rightarrow \infty$

$$\frac{\hbar\omega}{2kT} \rightarrow \text{small}$$

$$\coth x \sim \frac{1}{x} \quad x \ll 1$$

$$\Rightarrow \coth \frac{\hbar\omega}{2kT} \rightarrow \frac{2kT}{\hbar\omega}$$

$$U = \frac{3}{2} N\hbar\omega \coth \frac{\hbar\omega}{2kT}$$

$$T \approx_{\text{large}} \frac{3}{2} N\hbar\omega \frac{2kT}{\hbar\omega} = 3NkT$$

This agrees with classical calculation and equipartition theorem

When  $T \rightarrow 0$

$$\coth x \rightarrow 1 \text{ when } x \rightarrow \infty$$

Hence

$$\begin{aligned} U \approx_{\text{t-small}} \frac{3}{2} N\hbar\omega \times (1) \\ &= \frac{3}{2} N\hbar\omega \end{aligned}$$

Remember

$$\begin{aligned} \hat{\epsilon}_k &= \hbar\omega \left( k + \frac{1}{2} \right) \\ k &= 0, 1, 2, \dots \end{aligned}$$

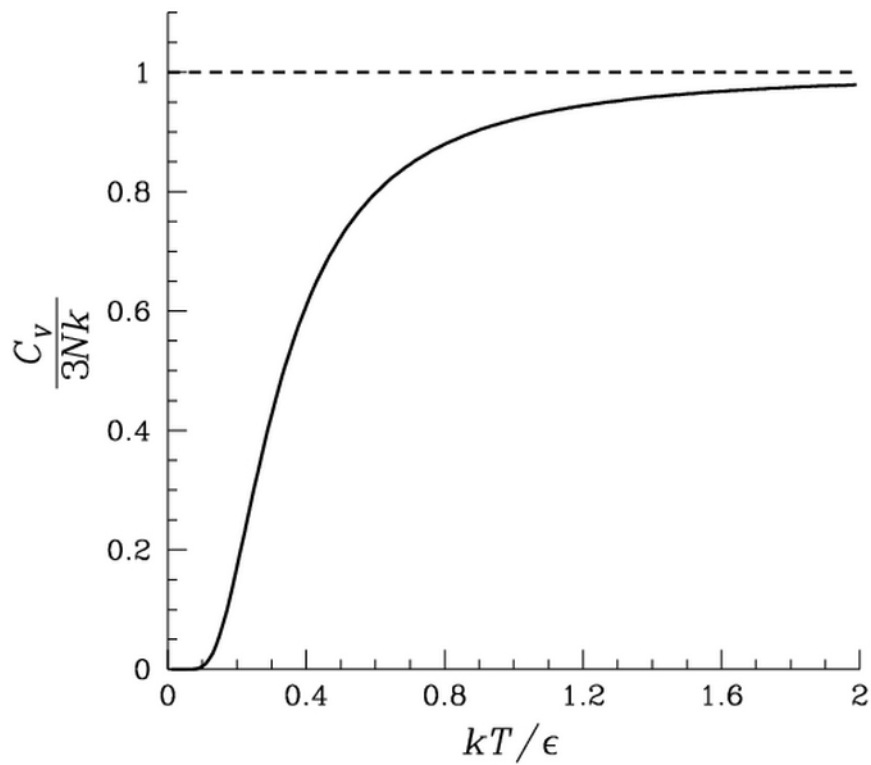
$$\hat{\epsilon}_0 = \frac{\hbar\omega}{2}$$

At very low T

At very low T, virtually all the oscillators are in the ground state!

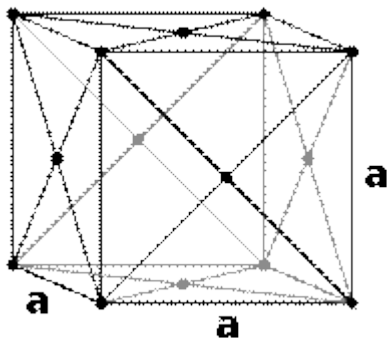
Also

$$C_v = \frac{\delta U}{\delta T} = \begin{cases} 3Nk & (T \rightarrow \infty) \\ 0 & (T \rightarrow 0) \end{cases}$$



$$C_v = 3Nk \left( \frac{\frac{\hbar\omega}{2kT}}{\sinh \frac{\hbar\omega}{2kT}} \right)^2$$

Good: QM calculation explains the fact that equipartition does not hold at low T



In a real solid, the interactions (i.e. potential) cannot be reduced to 3N copies of oscillator, All with same frequency  $\omega$ ! Many different values of  $\omega$  to be used. (interaction between all particles)

In practice: our H is too simple to fit the data



# Grand Canonical ensemble

30 November 2011

09:31

Remember that:

Density function  $\rho$  chosen on the basis of a set of constraints which define ensemble

*Microcanonical*                      *Canonical*

→

*E, N fixed*                      *T, N Fixed*

↓                                      ↓

$$\rho = \begin{cases} 1 & E < H < E + \Delta \\ 0 & \text{otherwise} \end{cases} \quad \rho = e^{-\beta H}$$

What does  $e^{-\beta H}$  mean?

- At fixed T ( $\beta$ ) states with lower energy are more important
- At lower T, the difference in the weight is very large

$\beta$ : parameter encodes thermal ("disorder") fluctuations

H: classical dynamics

However: Keeping N fixed is unrealistic!

## Grand Canonical

Constraints are ( $T, \mu$ ) are fixed

$\mu$  = chemical potential

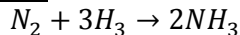
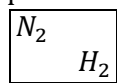
Replaces the role of N in the construction

In general, we expect

$$F = F(T, V, N)$$

$$\mu \equiv \left( \frac{\delta F}{\delta N} \right)_{V, T}$$

Example



Generalize thermodynamic potentials

$$dF = -S dT - P dV + \mu dN$$

$$dU = T dS - P dV + \mu dN$$

## Grand Canonical Ensemble

N allowed to vary

Define density function

$$\rho(N, q, p) \equiv \frac{z^N}{N! h^{3N}} \exp[-\beta PV - \beta H]$$

N=discrete parameter

p,q=for each choice of there are  $3N q_i$  and  $3N p_i$

P=pressure

Fugacity

$$z \equiv e^{\beta \mu}$$

$$\beta \equiv \frac{1}{kT}$$

$\mu$  = chemical potential

Define Grand Partition Function

$$Z \equiv \sum_{N=0}^{\infty} z^N Z_N$$

$Z_N$  = partition function

Equation of state

$$\ln Z = \frac{PV}{kT}$$

All other interesting thermodynamic quantities compute via ensemble averages

Derivation

2 systems

$$N_1 \ll N_2 = N - N_1$$

$$V_1 \ll V_2 = V - V_1$$

Systems at equilibrium with each other

Same T

But in general, we allow them to exchange particles

Partition function of (1)+(2) (two systems)

(set  $h=1$ )

$$Z_N = \int \left( \frac{d^{3N} q d^{3N} p}{N!} \right) e^{-\beta H}$$

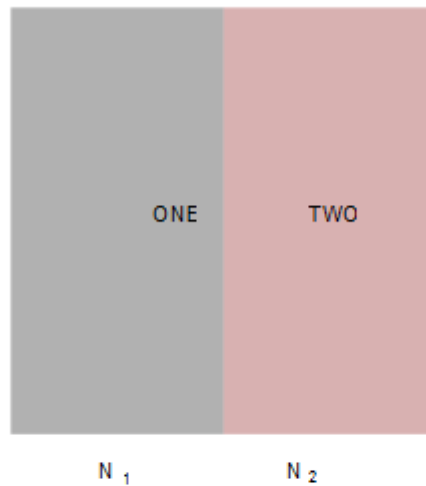
Assume that  $H = H_1 + H_2$

(no interaction terms between 1 and 2)

$$= \sum_{N_1=0}^N \frac{N!}{N_1! N_2!} \int \left( \frac{d^{3N_1} q_1 d^{3N_1} p_1 d^{3N_2} q_2 d^{3N_2} p_2}{N!} \right) e^{-\beta(H_1+H_2)}$$

$$d^{3N} q d^{3N} p$$

$$= dq_1 dq_2 dq_3 \dots dq_{3N_1} dq_{3N_1+1} \dots dq_{3N} \times dp_1 dp_2 dp_3 \dots dp_{3N_1} dp_{3N_1+1} \dots dp_{3N}$$



$dq_1 dq_2 dq_3 \dots dq_{3N_1}$  and  $dp_1 dp_2 dp_3 \dots dp_{3N_1}$  correspond to 1, others correspond to two

$$= \sum_{N_1=0}^N \int \frac{d^{3N_1} q_1 d^{3N_1} p_1}{N_1!} e^{-\beta H_1} \int \frac{d^{3N_2} q_2 d^{3N_2} p_2}{N_2!} e^{-\beta H_2}$$

$$N_2 = N - N_1$$

$$= \sum_{N_1=0}^N \int \frac{d^{3N_1} q_1 d^{3N_1} p_1}{N_1!} e^{-\beta H_1} Z_{N-N_1} = Z_N$$

$$1 = \sum_{N_1} \int \frac{d^{3N_1} q_1 d^{3N_1} p_1}{N_1!} e^{-\beta H_1} \frac{Z_{N_2}}{Z_N}$$

$$F_N \equiv kT \ln Z_N$$

$$1 = \sum_{N_1=0}^N \int \frac{d^{3N_1} q_1 d^{3N_1} p_1}{N_1!} e^{-\beta H_1} e^{-\beta(F_{N_2} - F_N)}$$

Taylor expand for small  $N_1 = N - N_2$

$$F_{N_2} - F_N = F(V - V_1, T, N - N_1) - F(V, T, N)$$

$$\approx \frac{\delta F}{\delta V} (\Delta V) + \frac{\delta F}{\delta N} (\Delta N)$$

$$= (-P)(-V_1) + \mu(-N_1)$$

$$F_{N_2} - F_N = PV_1 - \mu N_1$$

$$1 = \sum_{N_1=0}^N \int \frac{d^{3N_1} q_1 d^{3N_1} p_1}{N_1!} e^{-\beta H_1} e^{-\beta(PV_1 - \mu N_1)}$$

P has no index because systems are in mechanical equilibrium (same pressure)

$e^{-\beta(PV_1 - \mu N_1)}$  does not depend on  $(q_1, p_1)$

$$= \sum_{N_1=0}^N e^{-\beta(PV_1 - \mu N_1)} Z_{N_1}$$

Now take  $N \rightarrow \infty$  and drop the "1"

$$1 = \sum_{N=0}^{\infty} e^{-\beta PV} e^{\beta \mu N} Z_N$$

$e^{-\beta PV}$  = no N dependence

$$= e^{-\beta PV} \sum_{N=0}^{\infty} z^N Z_N$$

$$z^N Z_N = Z$$

(grand partition function)

$$= e^{-\beta PV} Z$$

$$\Rightarrow \boxed{\frac{PV}{kT} = \ln Z}$$

Average number of particles:

Def. ensemble average

$$\langle N \rangle = \frac{\sum_N z^N Z_N N}{\sum_N z^N Z_N}$$

Because  $Z_N$  does not depend on  $z$ ,

$$\langle N \rangle = \frac{\delta}{\delta z} \frac{\sum_N z^N Z_N}{\sum_N z^N Z_N}$$

$$= \frac{\delta}{\delta z} Z$$

$$= \frac{\delta}{\delta z} \ln Z$$

$$\boxed{\langle N \rangle = z \frac{\delta}{\delta z} \ln Z(z, V, T)}$$

Internal energy

$$U = E = \langle H \rangle$$

$$= \frac{\delta}{\delta \beta} \ln Z$$

Proof

$$-\frac{\delta}{\delta \beta} \ln Z = -\frac{\delta}{\delta \beta} \ln \sum_N z^N Z_N$$

$$= -\frac{\delta}{\delta \beta} \ln \sum_N z^N \int$$

.....

$$= -\left( \frac{\delta}{\delta \beta} \left( \sum_N z^N \int \frac{d^{3N} q d^{3N} p}{N!} e^{-\beta H} \right) \right) / \left( \sum_N z^N \int \frac{d^{3N} q d^{3N} p}{N!} \right)$$

.....

Monoatomic ideal gas

$$H = \frac{1}{2m} \sum_i p_i^2$$

We already know that

$$Z_N = \frac{(cVT^{\frac{3}{2}})^N}{N!}$$

Also, let us compute

$$\begin{aligned} Z &= \sum_{N=0}^{\infty} z^N Z_N \\ &= \sum_{N=0}^{\infty} \frac{(czVT^{\frac{3}{2}})^N}{N!} \\ &= \exp[czVT^{\frac{3}{2}}] \end{aligned}$$

Equation of state

$$\frac{PV}{kT} = \ln Z = czVT^{\frac{3}{2}}$$

Compute  $\langle N \rangle$

$$\begin{aligned} \langle N \rangle &= z \frac{\delta}{\delta z} \ln Z \\ &= z \frac{\delta}{\delta z} (czVT^{\frac{3}{2}}) \\ &= czvT^{\frac{3}{2}} = \ln Z \end{aligned}$$

Go back to E.O. state

$$\frac{PV}{kT} = \ln Z = \langle N \rangle$$

$$\Rightarrow \boxed{PV = \langle N \rangle kT}$$

Internal energy

$$\begin{aligned} U = \langle H \rangle &= -\frac{\delta}{\delta \beta} \ln Z \\ &= -\left(\frac{\delta \beta}{\delta T}\right)^{-1} \frac{\delta}{\delta T} \ln Z \\ &= \left(-\frac{1}{kT}\right)^{-1} \frac{\delta}{\delta T} (czVT^{\frac{3}{2}}) \\ &= \frac{3}{2} kT T czVT^{\frac{1}{2}} \\ &= \frac{3}{2} kT (czVT^{\frac{3}{2}}) \\ &= \boxed{\frac{3}{2} \langle N \rangle kT = U} \end{aligned}$$

Quantum Gas Distributions

Grand canonical treatment

Basic QM principles

- 1) Energy levels of many systems are discrete

e.g.

Particle in a box 1-D

$$\hat{s}_m = \frac{\hbar^2 m^2}{8mL}$$

Harmonic oscillator

$$\hat{E}_m = \hbar\omega \left(m + \frac{1}{2}\right)$$

...

- 2) Because identical particles are not distinguishable then

If 1- particle states are

$$\psi_1(x_1)$$

$$\psi_2(x_1)$$

The 2-particle state is NOT  $\psi_1(x_1)\psi_2(x_1)$

How to build 2-particle states?

In nature, there exist two kinds of particles: Bosons, Fermions

- Bosons:

The state of N-particles is symmetric under exchange of any two particles

Example:  $\psi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)$

.....

- Fermions:

Example  $\psi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)$

Fermions obey Pauli exclusion principle: two identical fermions cannot occupy the same state

Proof

"same state" means that the function

$$\psi_1(x) = \psi_2(x) \equiv \phi(x)$$

$$\psi(x_1, x_2) = \phi(x_1)\phi(x_2) - \phi(x_2)\phi(x_1) = 0$$

Spin statistics theorem fermions have half-integer spin, while bosons have integer spin

Fermions: electrons, quark, neutrinos, muon, protons, neutron, ...

Bosons: photon, W, Z, Gluon

- We call level the single particle energy eigenstate

$\hat{\epsilon}_i$ : *i* label state

Total energy of N particles

$$E = \sum_{k=1}^N \hat{\epsilon}_{ik}$$

*i* = state

*k* = label of particle

- We call occupation number  $\hat{m}_i$  the number of particles in energy level  $\hat{\epsilon}_i$

$$E = \sum_{i=0}^{\infty} \hat{m}_i \hat{\epsilon}_i$$

- We can describe a microscopic state in terms of the sequence of occupation numbers

$$\{\hat{m}_k\} \equiv \{\hat{m}_0, \hat{m}_1, \hat{m}_2, \dots, \hat{m}_N \dots\}$$

Consider a gas of particles occupying volume V at equilibrium with temperature T, and compute the Grand Canonical Ensemble

$$Z \equiv \sum_{N=0}^{\infty} z^N Z_N$$

N = number of functions

$z = e^{-\beta\mu}$  = fugacity

$Z_N$  = Partition function

$$= \sum_N z^N \sum_{\{\hat{m}_k\}} e^{-\beta \sum_k \hat{m}_k \hat{\epsilon}_k}$$

$\sum_N$  = sum over different number of particle

$\sum_k$  = sum over levels

$\sum_{\{\hat{m}_k\}}$  = sum over all possible sequences of occupation number subject to the

constraint  $\sum_{k=0}^{\infty} \hat{m}_k = N$

Our first task is to solve constraint!

$$\begin{aligned}
&= \sum_N \sum_{\{\hat{m}_k\}} z^{\sum_k \hat{m}_k} e^{-\beta \sum_k \hat{m}_k \hat{\epsilon}_k} \\
&= \sum_N \sum_{\{\hat{m}_k\}} e^{-\beta \sum_k \hat{m}_k (\hat{\epsilon}_k - \mu)} \\
&= \sum_{\{\hat{m}_k\}} e^{-\beta \sum_k \hat{m}_k (\hat{\epsilon}_k - \mu)} \\
&\quad \{\hat{m}_k\} \leftarrow \text{no constraints} \\
&= \sum_{\{\hat{m}_k\}} \prod_k [e^{-\beta(\hat{\epsilon}_k - \mu)}]^{\hat{m}_k} \\
&= \sum_{\hat{m}_0} \sum_{\hat{m}_1} \sum_{\hat{m}_2} \dots [e^{-\beta(\hat{\epsilon}_k - \mu)}]^{\hat{m}_0} [e^{-\beta(\hat{\epsilon}_k - \mu)}]^{\hat{m}_1} \dots \\
&= \prod_{k=0} \left[ \sum_{\hat{m}_k=0} [e^{-\beta(\hat{\epsilon}_k - \mu)}]^{\hat{m}_k} \right]
\end{aligned}$$

We managed to carefully rewrite Z as summations done level-by-level

# Quantum gas

14 December 2011

09:16

Grand canonical ensemble

$$Z = \sum_N z^N Z_N$$

$$= \prod_{k=0}^{\infty} \left[ \sum_{\hat{m}_k=0}^{\infty} [\exp -\beta(\hat{\epsilon}_k - \mu)]^{\hat{m}_k} \right]$$

k=levels  
 $\hat{m}_k$  = occupation number of level  
 NO CONSTRAINTS

Fermion

$$\hat{m}_k = 0,1$$

$$\sum_{\hat{m}_k} [e^{-\beta(\hat{\epsilon}_k - \mu)}]^{\hat{m}_k} = [e^{-\beta(\hat{\epsilon}_k - \mu)}]^0 + [e^{-\beta(\hat{\epsilon}_k - \mu)}]^1 = 1 + e^{-\beta(\hat{\epsilon}_k - \mu)}$$

$$Z = \prod_{k=0}^{\infty} [1 + e^{-\beta(\hat{\epsilon}_k - \mu)}]$$

Equation of state

$$\frac{PV}{kT} = \ln Z = \ln \prod_{k=0}^{\infty} [1 + e^{-\beta(\hat{\epsilon}_k - \mu)}]$$

$$= \sum_k \ln(1 + e^{-\beta(\hat{\epsilon}_k - \mu)})$$

k=levels

Occupation number  $z^N = e^{\beta\mu}$ : Fugacity

$$\langle N \rangle = \sum_k \langle n_k \rangle$$

Average total number of particles in terms of average occupation numbers

$$\langle N \rangle = z \frac{\delta}{\delta z} \ln Z$$

$$= z \frac{\delta}{\delta z} \sum_k \ln(1 + ze^{-\beta\hat{\epsilon}_k})$$

$$= \sum_k \left( z \frac{1}{1 + ze^{-\beta\hat{\epsilon}_k}} \right)$$

By comparing term by term

$$\langle \hat{m}_k \rangle = \frac{1}{1 + e^{\beta(\hat{\epsilon}_k - \mu)}}$$

Fermi-Dirac Distribution

Bosons

$$\hat{m}_k = 0,1,2,3, \dots$$

$$\sum_{\hat{m}_k=0}^{\infty} (e^{-\beta(\hat{\epsilon}_k - \mu)})^{\hat{m}_k} = (e^{-\beta(\hat{\epsilon}_k - \mu)})^0 + (e^{-\beta(\hat{\epsilon}_k - \mu)})^1 + (e^{-\beta(\hat{\epsilon}_k - \mu)})^2 + (e^{-\beta(\hat{\epsilon}_k - \mu)})^3 + \dots$$

GEOMETRIC SERIES!

$$= \frac{1}{1 - e^{-\beta(\hat{\epsilon}_k - \mu)}}$$

$$Z = \sum_k \frac{1}{1 - e^{-\beta(\hat{\epsilon}_k - \mu)}}$$

Eq state

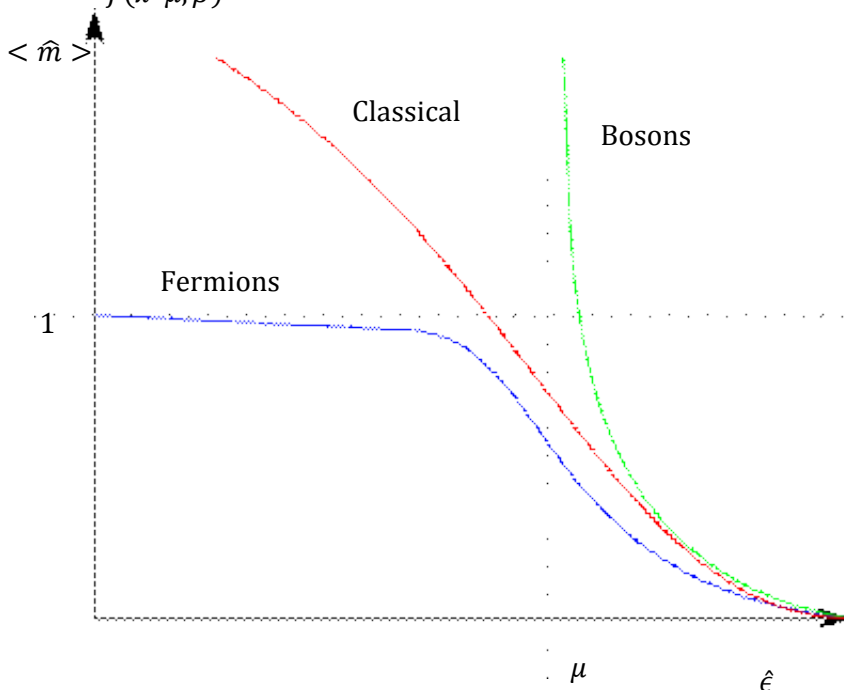
$$\begin{aligned}
\frac{PV}{kT} &= \ln Z = - \sum_k \ln(1 - e^{-\beta(\hat{\epsilon}_k - \mu)}) \\
\langle N \rangle &= z \frac{\delta}{\delta z} \ln Z \\
&= z \frac{\delta}{\delta z} \left[ - \sum_k \ln(1 - e^{-\beta \hat{\epsilon}_k}) \right] \\
&= \sum_k (-z) \frac{1}{1 - e^{-\beta \hat{\epsilon}_k}} (-e^{-\beta \hat{\epsilon}_k}) \\
&= \sum_k \frac{ze^{-\beta \hat{\epsilon}_k}}{1 - e^{-\beta \hat{\epsilon}_k}}, z = e^{\beta \mu} \\
&= \sum_k \frac{e^{-\beta(\hat{\epsilon}_k - \mu)}}{1 - e^{-\beta(\hat{\epsilon}_k - \mu)}} \\
&= \sum_k \frac{e^{-\beta(\hat{\epsilon}_k - \mu)} \times 1}{e^{-\beta(\hat{\epsilon}_k - \mu)} [e^{\beta(\hat{\epsilon}_k - \mu)} - 1]} \\
&= \sum_k \frac{1}{-1 + e^{\beta(\hat{\epsilon}_k - \mu)}}
\end{aligned}$$

$$\langle \hat{m}_k \rangle = \frac{1}{-1 + e^{\beta(\hat{\epsilon}_k - \mu)}}$$

Bose-Einstein distribution

$$\langle \hat{m}_k \rangle = \frac{1}{e^{\beta(\hat{\epsilon}_k - \mu)} + s}$$

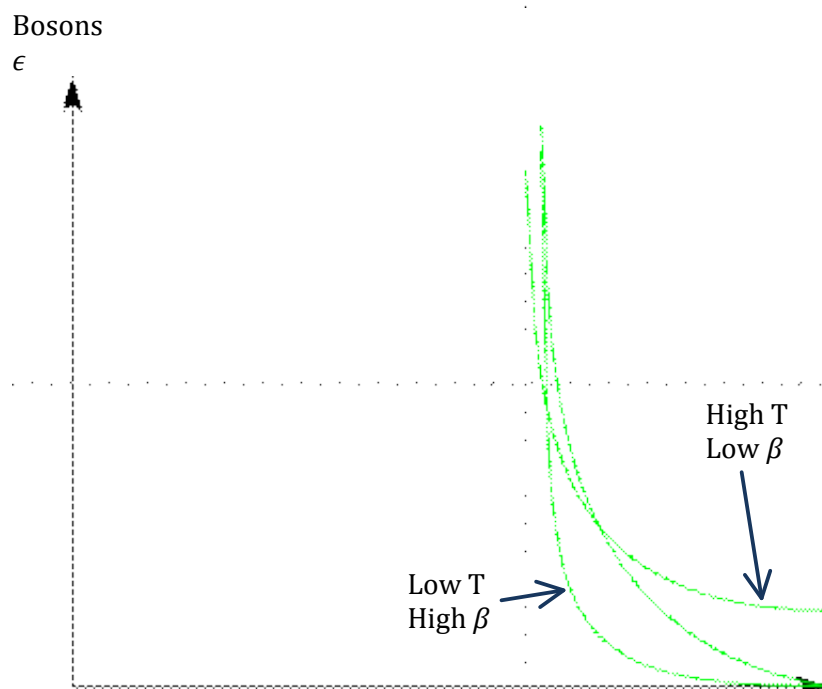
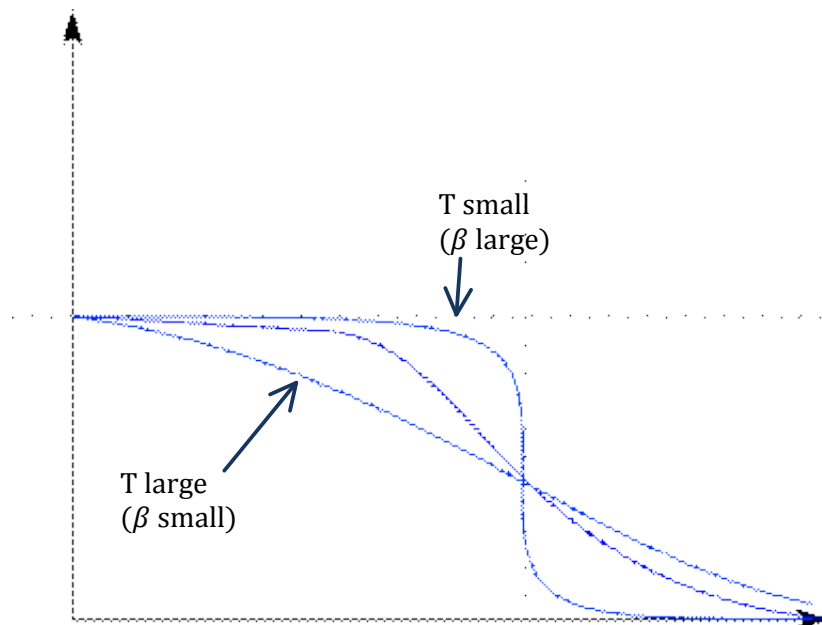
$s = -1$  for bosons (Bose-Einstein)  
 $s = +1$  for fermions (Fermi-Dirac)  
 $s = 0$  for semi-classical (Maxwell-Boltzmann)  
 $f(x, \mu, \beta)$



Fixed change  $\beta$   
Fermions

$\mu$





To summarise

1. Derived Quantum Gas distributions (with G. Canonical
2. At large T, or at large energy, all distributions agree with classical mechanics in physics
3. At low-T, huge differences appear
  - Bosons, fermions completely different

# Homework

15 December 2011

09:08

## Relativistic GAS

$$H_i = cP_i$$

i=1,...,N  
N=number particles

$$P_i \equiv \sqrt{P_{i1}^2 + P_{i2}^2 + P_{i3}^2}$$

$$H = \sum_{i=1}^N H_i$$

Set h=1, compute partition function

$$\begin{aligned} Z_N &= \frac{1}{N!} \int d^{3N}q d^{3N}p e^{-\beta H} \\ &= \frac{1}{N!} \int d^3p_1 d^3q_1 e^{-\beta H_1} d^3p_2 d^3q_2 e^{-\beta H_2} d^3p_3 d^3q_3 \dots \\ &= \frac{1}{N!} [\int d^3p_1 d^3q_1 e^{-\beta H_1}]^N \\ &\quad \text{Polar coordinates in } \bar{P}_1 \\ &\quad d^3p_1 = d\theta d\phi dp_1 p_1^2 \sin\theta \\ &\quad \int d\theta d\phi \sin\theta = 4\pi \\ &\quad H_i \text{ does not depend on coordinates } \bar{q}_1 \\ &\quad \int d^3q_1 = V \\ &= \frac{1}{N!} (4\pi V)^N [\int dp p^2 e^{-\beta cp}]^N \\ &\quad \int_0^\infty dx x^2 e^{-gx} = \frac{2}{g^3} \\ &= \frac{(4\pi V)^N}{N!} \left[ \frac{2}{\beta^3 c^3} \right]^N \\ &= \frac{(4\pi V)^N}{N!} \left[ \frac{2k^3 T^3}{c^3} \right]^N \\ &= \frac{(c_0 VT^3)^N}{N!} \end{aligned}$$

$$\begin{aligned} F &= -kT \ln Z_N \\ &= -kT \ln \frac{(c_0 VT^3)^N}{N!} \\ &= -NkT \ln c_0 VT^3 + kT \ln N! \\ &= -NkT \ln(c_0 VT^3) + kT (N \ln N - N) \\ &= -NkT [\ln(c_0 VT^3) - \ln N + 1] \\ &\quad 1 = \ln e \\ &= -NkT \left[ \ln \frac{c_0 VT^3 e}{N} \right] \\ &\quad \text{Since } c_0 \text{ is arbitrary constant, } c_0 \rightarrow ec_0 \\ &= -NkT \ln \frac{c_0 VT^3}{N} \end{aligned}$$

Pressure

$$\begin{aligned} P &= -\frac{\delta F}{\delta V} \\ &= -\frac{\delta}{\delta V} \left[ -NkT \ln \frac{c_0 VT^3}{N} \right] \\ &= \frac{NkT}{V} \end{aligned}$$

Entropy

$$S = -\frac{\delta F}{\delta T}$$

$$= -\frac{\delta}{\delta T} \left[ -NkT \ln \frac{c_0 VT^3}{N} \right]$$

$$= -\frac{F}{T} + 3Nk$$

Internal energy

$$U = F + Ts$$

$$= F + T \left( -\frac{F}{T} + 3Nk \right)$$

$$= 3NkT$$

Specific Heat

$$C_v = \frac{\delta U}{\delta T} = 3Nk$$

This result does NOT agree with the naïve version of the equipartition theorem because it does NOT depend quadratically on P!

However: it does agree with the generalized equipartition theorem

$$\left\langle x_i \frac{\delta H}{\delta x_j} \right\rangle = kT \delta_{ij}$$

$$H = H(x_i)$$

← p, q, e, ...

Then

$$x \frac{\delta H}{\delta x} = 2x^2 = 2H$$

$$\langle H \rangle = \frac{1}{2} \left\langle x \frac{\delta H}{\delta x} \right\rangle = \frac{1}{2} kT$$

Sum over all phase-space variable that enter quadratically

In exercise

$$H = cp$$

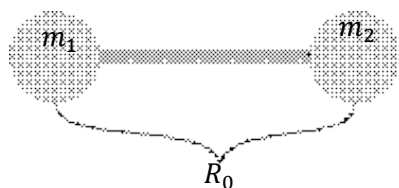
$$P \frac{\delta}{\delta P} H = cp = H$$

Exercise

N molecules of same diatomic gas with

$$H_i = \frac{1}{2m} P_i^2 + \frac{1}{2I} l_i^2 + \frac{1}{2\mu} P_i^2 + \frac{1}{2} \mu \omega^2 (R - R_0)^2$$

$$\frac{1}{2\mu} P_i^2 + \frac{1}{2} \mu \omega^2 (R - R_0)^2 \rightarrow \text{vibrational modes}$$



Phase-space for each molecule

$$\{\bar{P}, \bar{Q}, \bar{l}, \theta, \phi, R, \phi\}$$

$$12 = 3 \ 3 \ 2 \ 1 \ 1 \ 1 \ 1$$

$$\{p_1, q_1, P_2, q_2\}$$

$$\int d^{3N} Q$$

$$d^{3N} Q \ d^{3N} P \ d^{2N} L \ d^N \theta \ d^N \phi \ d^N R \ d^P \times (\sin \theta R^2)^N$$

Compute  $Z_N$

$$T^{\frac{3}{2}} T^3 T^{\frac{5}{3}}$$