* Lectures 4-5 *

– Introduction to QM –

Classical mechanics

Particle mechanics

Newton's equation

$$m\ddot{\vec{r}} = \vec{F} \qquad \vec{r}(t) = \text{instantaneous particle position}$$

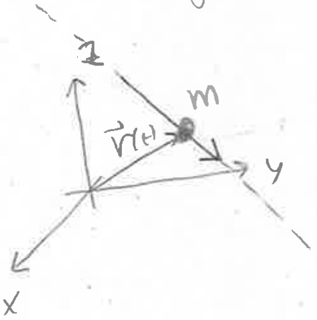
$$\begin{cases} m\ddot{x}(t) = F_x(\vec{r}(t)) \\ m\ddot{y}(t) = F_y(\vec{r}(t)) \\ m\ddot{z}(t) = F_z(\vec{r}(t)) \end{cases}$$

For a free particle $\vec{F} = 0$

and $\vec{r}(t) = \vec{r}_0 + \vec{v}t$

where $\vec{r}_0 = \vec{r}(t=0)$

$\vec{v} = \dot{\vec{r}}(t=0)$



Wave mechanics

Wave equation for SOUND waves, LIGHT waves, and WATER waves

For light:

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} - \frac{\partial^2 u}{\partial z^2} = 0$$

$u = u(x,y,z,t)$ = amplitude of the wave.

In 1D $\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0 \Rightarrow$

$\Rightarrow u(x,t) = a_+ f(x+ct) + a_- f(x-ct)$

If we know $u(x,0) = f(x)(a_+ + a_-)$, then

and $\dot{u}(x,0) = c f'(x)(a_+ - a_-)$

$$\begin{cases} a_+ = \frac{u(x,0)}{f(x)} + \frac{\dot{u}(x,0)}{cf'(x)} \\ a_- = \frac{u(x,0)}{f(x)} - \frac{\dot{u}(x,0)}{cf'(x)} \end{cases}$$

In the wave equation the position vector $\vec{r}$ is just a set of three parameters, x,y,z, upon which the amplitude u depends on.

To find the solutions of

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0 \qquad (1)$$

we use the Fourier Transform:

$$u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} v(k,t)\, e^{ikx}\, dk$$

then

$$\frac{\partial u}{\partial x} = \frac{1}{\sqrt{2\pi}}\int v(k,t)(ik)\, e^{ikx}\, dk$$

$$\begin{cases} \dfrac{\partial^2 u}{\partial x^2} = \dfrac{-1}{\sqrt{2\pi}}\displaystyle\int v(k,t)\, k^2 e^{ikx}\, dk \\[2ex] \dfrac{\partial^2 u}{\partial t^2} = \dfrac{1}{\sqrt{2\pi}}\displaystyle\int \ddot{v}(k,t)\, e^{ikx}\, dk \end{cases}$$

$$(1) \to \frac{1}{\sqrt{2\pi}}\int \left(\frac{1}{c^2}\frac{\partial^2 v}{\partial t^2} + k^2 v\right) e^{ikx}\, dk = 0 \quad \Rightarrow$$

$$\Rightarrow \quad \frac{\partial^2 v(k,t)}{\partial t^2} + c^2k^2 v(k,t) = 0 \quad \Rightarrow \boxed{v(k,t) = A(k)\, e^{ickt} + B(k)\, e^{-ickt}}$$

$$\to \quad u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[A(k)\, e^{ik(x+ct)} + B(k)\, e^{ik(x-ct)}\right] dk$$

right-propagating

How to determine A and B?

We know that:

$$u(x,0) = \frac{1}{\sqrt{2\pi}}\int \left[A(k) + B(k)\right] e^{ikx}\, dk$$

$$\dot{u}(x,0) = \frac{ic}{\sqrt{2\pi}} \int [A(k) - B(k)]\, k\, e^{ikx}\, dx$$

By def: of FT

$$A(k) + B(k) = \frac{1}{\sqrt{2\pi}} \int u(x,0)\, e^{-ikx}\, dx$$

$\Rightarrow$ Take sum and difference:

$$[A(k) - B(k)]\, cki = \frac{1}{\sqrt{2\pi}} \int \dot{u}(x,0)\, e^{-ikx}\, dx$$

$$A(k) = \frac{1}{2\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[u(x,0) - \frac{i}{ck}\dot{u}(x,0)\right] e^{-ikx}\, dx$$

$$B(k) = \frac{1}{2\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[u(x,0) + \frac{i}{ck}\dot{u}(x,0)\right] e^{-ikx}\, dx$$

Homework – Calculate $A(k)$ and $B(k)$ for

$$u[x\_, t\_] := \alpha\, e^{-\frac{1}{2}(x+ct)^2\alpha^2 + i\,a\,(x+ct)} + \beta\, e^{-\frac{1}{2}(x-ct)^2\beta^2 + i\,b\,(x-ct)}$$

Sol:

$$A(k) = \exp\left[-\frac{(k-a)^2}{2\alpha^2}\right]$$

$$B(k) = \exp\left[-\frac{(k-b)^2}{2\beta^2}\right]$$

Quantum mechanics

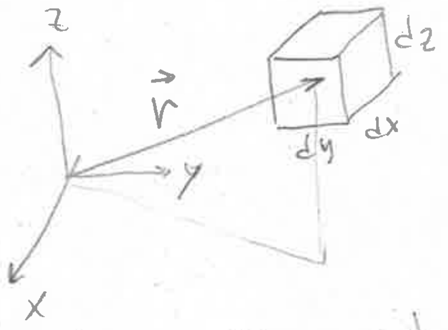
In QM (non-relativistic theory) the state of one particle can be described, at a given time, by a (in general complex) function of the coordinates $\vec{r}$ of the particle

$$\psi(\vec{r})$$

such that: (Born's rule)

$$|\psi(\vec{r})|^2 dx\,dy\,dz$$

is equal to the PROBABILITY that a measurement of the position of the particle give the particle located in a volume $dV = dx\,dy\,dz$ about $\vec{r}$.



It must be necessarily normalized:

$$\underbrace{\int |\psi|^2 dV = 1}$$

Therefore the integral must converge.

$\psi(\vec{r})$ determine also the prob. of other measurements

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Esempio: qual è la prob che dato $\psi(x)$ trovo l'impulso p?
La risposta è ovviamente

$$P = |\langle p|\psi\rangle|^2$$

dove $\langle p|\psi\rangle = \int dx \langle p|x\rangle\langle x|\psi\rangle = \int dx \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{ipx}{\hbar}} \psi(x)$

Perciò:

$$P = \int dx'\,dx\, \psi^*(x') \frac{e^{\frac{ipx'}{\hbar}}}{\sqrt{2\pi\hbar}} \psi(x) \frac{e^{-\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}} \qquad K(p|x,x') = \frac{e^{\frac{ip(x'-x)}{\hbar}}}{2\pi\hbar}$$

$$= \int dx'\,dx\, \psi^*(x')\, K(p|x,x')\, \psi(x)$$

these probs can always be written as:

Prob. of measuring "a" $= \int \psi^*(\vec{r})\, \underbrace{A(\vec{r},\vec{r}')}\, \psi(\vec{r}')\, d^3r\, d^3r'$

it depends on the kind of measurement.

VEDI 4-5.5 b

— Time —

The state of the system, and with it the wave function, in general varies with Time.

If at $t=0$ $\psi(\vec{r})$ is know, then $\psi(\vec{r},t)$ at a later time $t>0$ is <u>completely</u> determined by $\psi(\vec{r})$ <u>only</u> via the Schrödinger equation. For a <u>free</u> particle of mass m This is:

$$\boxed{i\hbar \frac{\partial \psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}\psi + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}\right]}$$

$\hbar$ = reduced Plank constant $= \frac{h}{2\pi}$ $\qquad E \cdot t = p x$

$\simeq 6.626\,070\,040(81) \times 10^{-34}$ J·s

It is a <u>first-order differential equation</u>!

In 1D:

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

· From

$$P = |\psi(\vec{r})|^2 dV$$

it follows the $\psi(\vec{r})$ and $\psi(\vec{r})e^{i\alpha(\vec{r})}$ with $\alpha(\vec{r}) \in \mathbb{R}$

give the same COORDINATE prob. distr

- More generally, from:

$$P(A) = \int \psi^*(\vec{r}) A(\vec{r}, \vec{r}') \psi(\vec{r}') \, dV dV'$$

it follows tha

$\psi(\vec{r})$ and $\psi(\vec{r})e^{i\beta}$ $\beta \in \mathbb{R}$, β = indep of $\vec{r}$

represents the SAME state

We <u>require</u> that $\psi(\vec{r})$ is a <u>continuous</u> function

We use again the Fourier method.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(k,t)\, e^{ikx}\, dk$$

$$0 = i\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{ikx}\left\{i\hbar\frac{\partial\phi(k,t)}{\partial t} - \frac{\hbar^2k^2}{2m}\phi(k,t)\right\}$$

Note that $[\hbar k] = \text{Energy} \times \frac{\text{time}}{\text{length}} = \frac{\text{Energy}}{\text{velocity}} = \frac{mv^{\cancel{2}}}{\cancel{v}} = mv = \underline{\text{momentum}}$

Kin. en $= \frac{1}{2}mv^2 \Rightarrow [E] = mv^2$

$$\boxed{i\hbar\frac{\partial\phi(k,t)}{\partial t} - \frac{\hbar^2k^2}{2m}\phi(k,t) = 0} \longrightarrow \phi(k,t) = \phi(k,0)\, e^{-i\left(\frac{\hbar^2k^2}{2m}\right)\frac{t}{\hbar}}$$

and $$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k,0)\, e^{-i\left(\frac{\hbar^2k^2}{2m}\right)t/\hbar}\, e^{ikx}\, dk$$

def $p = \hbar k \Rightarrow$ $$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\frac{\phi(p/\hbar,0)}{\sqrt{\hbar}}\, e^{-i\frac{p^2}{2m}t/\hbar + i\frac{px}{\hbar}}\, dp$$

choose $$\frac{\phi(p/\hbar,0)}{\sqrt{\hbar}} \propto \exp\left[-\frac{p^2}{2\Delta p^2}\right] \Rightarrow$$

$$\Rightarrow \boxed{\psi(x,t) \propto \sqrt{\frac{\Delta p^2}{\sigma(t)}}\,\exp\left[-\frac{mx^2}{2\sigma(t)/\Delta p^2}\right]}$$

$\sigma(t) = m\hbar^2 + it\hbar\Delta p^2$

$$\frac{\sigma(t)}{\Delta p^2} = \frac{m\hbar^2}{\Delta p^2} + it\hbar = m\left(\frac{\hbar^2}{\Delta p^2} + it\frac{\hbar}{m}\right) \equiv m\,\Delta x^2(t)$$

$$\Delta x^2(t) \equiv \frac{\sigma(t)}{m\Delta p^2} = \frac{\hbar^2}{\Delta p^2} + it\frac{\hbar}{m}$$

$p = m\frac{\ell}{t}$

$$\frac{\Delta p^2}{\sigma(t)} = \frac{1}{m\Delta x^2} \qquad \sim \frac{\cancel{p^2}x^2}{\cancel{p^2}} + i\frac{tpx}{\frac{pt}{\ell}} = \ell^2 \text{ ok!}$$

$$\Delta x^2(0) = \frac{\hbar^2}{\Delta p^2}$$

therefore $$\Delta x^2(t) = \frac{\hbar^2}{\Delta p^2}\left(1 + i\,\frac{t\,\cancel{\hbar}}{m}\,\frac{\Delta p^2}{\hbar^{\cancel{2}}}\right)$$

$$\boxed{\Delta x^2(t) = \frac{\hbar^2}{\Delta p^2}\left(1 + i\,\frac{\Delta p^2}{m}\,\frac{t}{\hbar}\right)}$$

$$\psi(x,t) = \sqrt{\frac{\hbar}{\Delta x^2(t)}}\;\exp\left[-\frac{x^2}{2\Delta x^2(t)}\right]$$

$$\Delta x(t) = \frac{\hbar}{\Delta p}\sqrt{1 + i\,\frac{\Delta p^2}{m}\,\frac{t}{\hbar}}$$

$$\mathrm{Re}\,\Delta x^2 = \frac{\hbar}{\Delta p} \equiv u$$

$$\mathrm{Im}\,\Delta x^2 = \frac{\Delta p\, t}{m} \equiv v$$

$$u^2 + v^2 = \frac{\hbar^2}{\Delta p^2} + \frac{\Delta p^2 t^2}{m^2} = \frac{\hbar^2}{\Delta p^2}\left(1 + \frac{\Delta p^4 t^2}{m^2 \hbar^2}\right)$$

$$|\psi(x,t)|^2 = \frac{\Delta p}{\sqrt{1 + \frac{\Delta p^4 t^2}{m^2\hbar^2}}} \;*$$

$$*\;\mathrm{Exp}\left[-\cancel{\frac{\hbar}{\Delta p}}\;\frac{1 \quad x^2}{\frac{\hbar^2}{\Delta p^2}\left(1 + \frac{\Delta p^4 t^2}{m^2\hbar^2}\right)}\right]$$

↑ the width increase wit time..

$$t_0^2 \equiv \frac{m^2\hbar^2}{\Delta p^4} = \frac{m^2 p^2 x^2}{p^4} = \frac{m^2 x^2}{p^2} = \frac{\cancel{m^2}\,\cancel{L^2}}{\cancel{m^2}\,\frac{\cancel{L^2}}{T^2}} = T^2$$

$$\boxed{|\psi(x,t)|^2 = \frac{\hbar}{\Delta x_0^2}\,\frac{1}{\sqrt{1 + t^2/t_0^2}} \;*\; \mathrm{Exp}\left[-\frac{x^2}{\Delta x_0^2\left(1 + \frac{t^2}{t_0^2}\right)}\right]}$$

$$\boxed{t_0 = \frac{m\hbar}{\Delta p^2} \qquad \Delta x_0 = \frac{\hbar}{\Delta p}}$$

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2\, dx = \sqrt{\frac{\pi}{\Delta x_0}}\;\hbar$$

$$\boxed{\psi(x,t) = \frac{1}{\sqrt{\sqrt{\pi}\,\Delta x_0\left(1 + i\frac{t}{t_0}\right)}}\;\mathrm{Exp}\left[-\frac{x^2}{2\Delta x_0^2\left(1 + i\frac{t}{t_0}\right)}\right]}$$

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{\Delta x_0^2 (1+\frac{t^2}{t_0^2})}} \operatorname{Exp}\left[-\frac{x^2}{\Delta x_0^2(1+\frac{t^2}{t_0^2})}\right]$$

Clearly $\Delta x^2(t) = \Delta x_0^2(1+t^2/t_0^2)$ grows with t

$\dot{\Delta x^2}(t) = \frac{2\Delta x_0^2}{t_0} t \Rightarrow \Delta x^2(t)$ grows QUICKER if

t_0 is <u>small</u>. BuT $t_0 = \frac{m\hbar}{\Delta p^2}$

If the mass is big, t_0 is big

If Δp is big (so Δx_0 is small $\Leftrightarrow$ localized particle)

then t_0 is small and the spread quick.

SCH. equation is <u>liner</u>. if $\hat{H} \equiv -\frac{\hbar^2}{2m}\Delta$

then $i\hbar \frac{\partial\psi}{\partial t} = \hat{H}\psi$ $\quad \hat{H}$ = Hamiltonian operator

Then if ψ_1 and ψ_2 are solution:

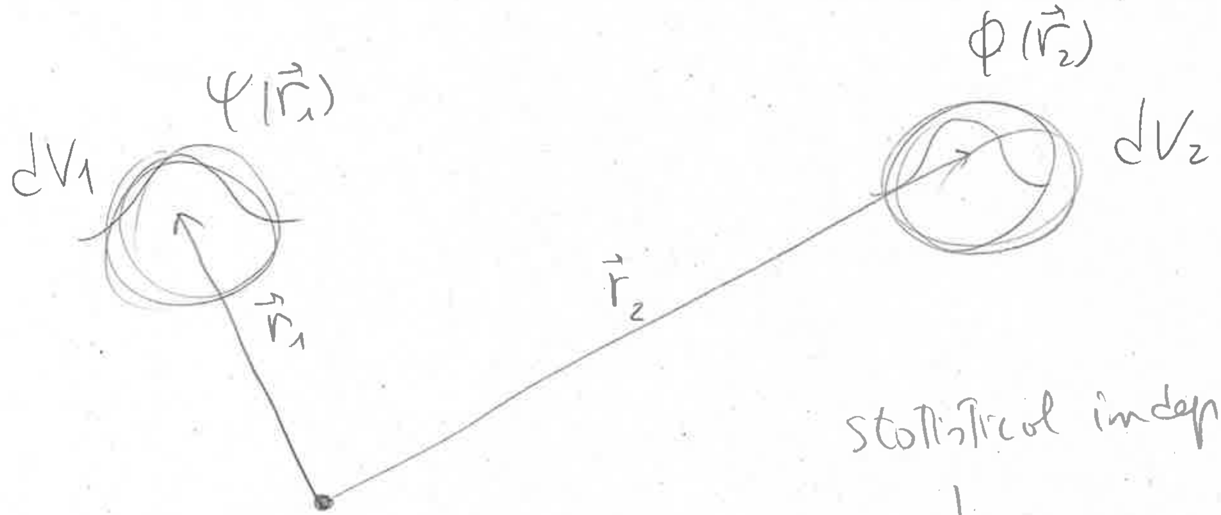
$$i\hbar \frac{\partial \psi_n}{\partial t} = \hat{H}\psi_n$$

then also $\psi = c_1\psi_1 + c_2\psi_2$ $\quad c_1, c_2 \in \mathbb{C}$

is a solution

.- 2 party sistems -

Consider two wave packets for gratt. of 2 particles



statistical indep.

↓

Then it is reasonable that:

$$dP(\vec{r}_1,\vec{r}_2)\,dV_1\,dV_2 = |\psi(\vec{r}_1)|^2 dV_1\,|\phi(\vec{r}_2)|^2 dV_2$$

and, therefore

$$\Psi(\underline{r}_1,\underline{r}_2) = \psi(\underline{r}_1)\,\phi(\underline{r}_2)$$

Moreover, if the particles do not interact, then:

$$\Psi(\underline{r}_1,\underline{r}_2,t) = \psi(\underline{r}_1,t)\,\phi(\underline{r}_2,t)$$

- Example - Two free particles in 1D

$$i\hbar\frac{\partial}{\partial t}[\psi(x_1,t)\,\phi(x_2,t)] = \left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right)[\psi(x_1,t)\cdot\phi(x_2,t)]\left(-\frac{\hbar^2}{2m}\right)$$

$$\Rightarrow \phi(i\hbar\dot{\psi})+\psi(i\hbar\dot{\phi}) = \phi\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x_1^2}\right)+\psi\left(-\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x_2^2}\right)$$ divide be $\phi\psi$

$$\underbrace{\frac{1}{\psi}\left(i\hbar\dot{\psi}+\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x_1^2}\right)}_{\text{function of } x_1}+\underbrace{\frac{1}{\phi}\left(i\hbar\dot{\phi}+\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x_2^2}\right)}_{\text{function of } x_2}=0$$

$\Rightarrow$ separately $=0$

So, in general, the SchrÖ eq for N particles is:

$$i\hbar \frac{\partial}{\partial t} \psi(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N, t) = (\hat{H}_1 + \hat{H}_2 + \cdots + \hat{H}_N)\, \psi(\underline{r}_1, \ldots, \underline{r}_N, t)$$

In our previous example, To ke

$$\phi(p,0) = \exp\left[-\frac{(p-p_0)^2}{2\Delta p^2}\right]$$

and

$$\psi(x,t) \propto \int_{-\infty}^{\infty} \phi(p,0)\, e^{-i\frac{p^2}{2m}\frac{t}{\hbar} + i p x}$$

$$= \sqrt{\frac{2\pi}{\Delta x_0^2 (1+i t/t_0)}}\ \hbar \exp\left[-\frac{\left(\frac{x}{\Delta x_0} - i\frac{p_0}{\Delta p}\right)^2}{2(1+i\, t/t_0)} - \frac{p_0^2}{2\Delta p^2}\right]$$

The normalized ψ is:

$$\psi(x,t) = \sqrt{\frac{1}{\sqrt{\pi}}\frac{1}{\Delta x_0 (1+i\frac{t}{t_0})}}\ \mathrm{Exp}\left[-\frac{1}{2}\frac{\left(\frac{x}{\Delta x_0} - i\frac{p_0}{\Delta p}\right)^2}{1+i\frac{t}{t_0}} - \frac{p_0^2}{2\Delta p^2}\right]$$

and

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{\pi}\,\Delta x_0}\frac{1}{\sqrt{1+\frac{t^2}{t_0^2}}} \exp\left[-\frac{\left(\frac{x}{\Delta x_0} - \frac{p}{\Delta p}\frac{t}{t_0}\right)^2}{1+t^2/t_0^2}\right]$$

The central value of the dist...

$$E[x] = \int_{-\infty}^{\infty} x\, |\psi(x,t)|^2\, dx = \Delta x_0 \frac{p_0}{\Delta p}\frac{t}{t_0} = \frac{p_0}{m} t$$

So, p_0 is related to the <u>momentum</u> of the particle

The variance is:

$$E[(x - \frac{p_0 t}{m})^2] = \frac{\Delta x_0^2}{2}\left(1 + \frac{t^2}{t_0^2}\right)$$ c.v.d