Matter waves of free particles

Particle $\left\{ \begin{array}{l} E = \hbar\omega \\ p = \hbar k \end{array} \right.$ what is the shape of a wave?

Plane wave in the +x direction:

(i) $\sin(kx - \omega t)$

(ii) $\cos(kx - \omega t)$

(iii) $e^{ikx - i\omega t}$ ($e^{-i\omega t}$ always)

(iv) $e^{-ikx + i\omega t}$ ($e^{+i\omega t}$ always)] phase.

Superposition + Probabilities:

↳ state of particle with the = prob. of moving to the left or right

(i) $\sin(kx - \omega t) + \sin(kx + \omega t) = 2\sin(kx)\cos(\omega t)$

but this vanishes at $(\omega t = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots)$

⇒ cannot be a matter particle.

ii) $\cos(kx - \omega t) + \cos(kx + \omega t) = 2\cos(kx)\cos(\omega t)$

Matter waves of free particles

iii) $e^{ikx-i\omega t} + e^{-ikx-i\omega t}$

$$= \left(e^{ikx} + e^{-ikx}\right) e^{-i\omega t} = 2\cos(kx)\, e^{-i\omega t}$$ (does not vanish)

(iv) $e^{-ikx} e^{i\omega t} + e^{ikx} e^{i\omega t}$

$$= 2\cos(kx)\, e^{i\omega t}$$ (does not vanish)

(iii) ∧ (iv) cannot be true at the same time.

Superimposing a state to itself does not change the state.

$$e^{ikx-i\omega t} + e^{-i(kx-\omega t)} = 2\cos(kx-\omega t)$$

energy part always has −

$$\Rightarrow \boxed{\Psi(x,t) = e^{ikx-i\omega t}} \text{ in 1D} \Rightarrow \Psi(\vec{r},t) = e^{i\vec{k}\vec{r}-i\omega t}$$

The above is the wave function for a particle with:

$p = \hbar k$

$E = \hbar\omega$

$\vec{p} = \hbar\vec{k}$

$E = \hbar\omega$

Wave function of a free particle

$\Psi(x,t) = e^{ikx - i\omega t}$ with $p = \hbar k$, $E = \hbar\omega$

Non-relativistic particles: $E = \frac{p^2}{2m}$

Momentum:

$$\left.\begin{aligned} &\underbrace{\frac{\hbar}{i}\frac{\partial}{\partial x}}\Psi = \hbar k \Psi = p\Psi \\ &\text{momentum operator: } \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \end{aligned}\right\} \Rightarrow \hat{p}\Psi = p\Psi$$

If this holds:

1) $\Psi(x,t)$ is an eigenstate of $\hat{p}$ with eigenvalue "p".

Remember: $\begin{bmatrix} \text{matrix} \end{bmatrix} \begin{bmatrix} \text{v} \\ \text{e} \\ \text{c} \\ \text{t} \\ \text{o} \\ \text{r} \end{bmatrix} = \alpha \begin{bmatrix} \text{v} \\ \text{e} \\ \text{c} \\ \text{t} \\ \text{o} \\ \text{r} \end{bmatrix}$

↳ rotate, same vector × constant

× ✓ eigenvector.

2) $\Psi(x,t)$ is a state of definite momentum.

Wave function of a free particle

Energy:

$$i\hbar \frac{\partial}{\partial t}\psi = i\hbar(-i\omega)\psi = \hbar\omega\psi = E\psi$$

We know that: $E = \frac{p^2}{2m}$, let's find an operator:

Then: $$E\psi = \frac{p^2}{2m}\psi = \frac{p}{2m}\underbrace{\hat{p}\psi}_{p\psi} = \frac{p}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\right) = \frac{1}{2m}\frac{\hbar}{i}\frac{\partial}{\partial x}(\underbrace{p\psi}_{\hat{p}\psi}) =$$

$$= \frac{1}{2m}\frac{\hbar}{i}\frac{\partial}{\partial x}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\right) = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\text{energy operator}}\psi$$

(2nd order PDE)

$$\boxed{\hat{E} = \frac{1}{2m}\hat{p}^2}$$

$\Rightarrow \hat{E}\psi = E\psi$

1) ψ is an eigenstate of $\hat{E}$.

2) ψ is a state of definite E.

Schrödinger equation of a free particle

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

Let's substitute this solution:

$$\psi = e^{ikx - i\omega t}$$

Into Schrödinger's equation:

$$i\hbar(-i\omega)\cancel{\psi} = -\frac{\hbar^2}{2m}(ik)^2\cancel{\psi}$$

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \Rightarrow \boxed{E = \frac{p^2}{2m}}$$

relation tells we have a particle plane wave that exists.

- Sln. is linear, so we can construct more general solutions.

The time-independent Schrödinger equation

How do we get $\Psi(x,t)$?

We need to solve Sch. eq:

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

for a specified potential $V = V(x,t)$

* For simplicity, we will assume that $V = V(x)$ is independent of t.

Then, we can use separation of variables, and look for solutions.

$$\Psi(x,t) = \psi(x)\,\varphi(t)$$

- Solutions of this type are only a subset, but they are interesting.
- We can patch together these solution to construct more general solutions.

The time-independent Schrödinger equation

Separation of variables: $$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

LHS:

$$\frac{\partial \Psi}{\partial t} = \psi(x) \frac{d\varphi(t)}{dt}$$

RHS:

$$\frac{\partial^2 \Psi}{\partial x^2} = \varphi(t) \frac{d^2 \psi}{dx^2}$$

ordinary derivatives

Sch. Eq:

$$\Rightarrow \quad i\hbar \psi \frac{d\varphi}{dt} = -\frac{\hbar^2}{2m} \varphi \frac{d^2\psi}{dx^2} + V\psi\varphi$$

$\div\ \psi\varphi$

$$\Rightarrow \quad \underbrace{i\hbar \frac{1}{\varphi} \frac{d\varphi}{dt}}_{\text{function of } t} = \underbrace{-\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2\psi}{dx^2} + V}_{\text{function of } x}$$

The time-independent Schrödinger equation

Separation of variables: $$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

Temporal ODE:

$$i\hbar \frac{1}{\varphi}\frac{d\varphi}{dt} = E$$

$$\Rightarrow \boxed{\frac{d\varphi}{dt} = -\frac{i}{\hbar} E\varphi} \text{ ODE} \Rightarrow \varphi(t) = C e^{-\frac{iE}{\hbar}t}$$

↗ the wiggle factor.

$$\varphi(t) = C\left(\cos\left(\frac{E}{\hbar}t\right) - i\sin\left(\frac{E}{\hbar}t\right)\right)$$

Spatial ODE:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E$$

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

time-independent Sch. equation.

* $V(x)$ needs to be specified.

Separable Solutions

Why are separable solutions important?

Most sln to time-depende S.eq do not take this form.

1) They are stationary states:

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

$$\Rightarrow |\Psi(x,t)|^2 = \Psi\Psi^* = \psi e^{-i\frac{E}{\hbar}t}\, \psi^* e^{+i\frac{E}{\hbar}t} = |\psi(x)|^2$$

the probability density does not depend on time.

Expectation Values:

$$\langle Q(x,p)\rangle = \int \Psi^* \left[Q\left(x, -i\hbar\frac{\partial}{\partial x}\right)\right] \Psi \, dx$$

$$\Rightarrow \langle Q(x,p)\rangle = \int \psi^* \left[Q\left(x, -i\hbar\frac{\partial}{\partial x}\right)\right] \psi \, dx$$

- Every expectation value is constant in time
- If $\langle x\rangle$ is constant, $\Rightarrow \langle p\rangle = 0$
- Nothing ever happens in a stationary state.

Separable Solutions

2) They are states of definite total energy.

$$H(x,p) = \frac{p^2}{2m} + V(x)$$ Hamiltonian.

The Hamiltonian operator is:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \quad \overset{\text{Sch eq}}{\Longrightarrow} \quad \hat{H}\psi = E\psi$$

The expectation value is:

$$\langle H \rangle = \int \psi^* \hat{H} \psi \, dx = E\int |\psi|^2 dx = E\int |\Psi|^2 dx = E$$

Also: $\hat{H}^2\psi = \hat{H}(\hat{H}\psi) = \hat{H}(E\psi) = E\hat{H}\psi = E^2\psi$

$$\Rightarrow \langle H^2 \rangle = \int \psi^* \hat{H}^2 \psi \, dx = E^2 \int |\psi|^2 dx = E^2$$

The variance of H is

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = E^2 - E^2 = 0 \quad \text{(zero spread)}$$

Every measurement of the total energy returns E in a separable sln.

Separable Solutions

3) The general solution is a linear combination of the separable slns.

$\psi_1(x), \psi_2(x), \psi_3(x) \Rightarrow \{\psi_n(x,t)\}$

$E_1 \quad E_2 \quad E_3 \qquad \{E_n\}$

$\Rightarrow \Psi_1(x,t) = \psi_1(x) e^{-i\frac{E_1}{\hbar}t}$, etc.

general $\Rightarrow$ solution

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}}}$$

Every sln. to the time-dependent S. eq can be written in this form. We need to find c_n.

Once you solved ψ $\Rightarrow$ getting a general sln. is straightforward.

Structure of a typical QM problem

We need to solve the time-dependent Schrödinger equation:

$$\left.\begin{array}{l} V(x) \\ \Psi(x,0) \end{array}\right\} \text{are given} \Rightarrow \Psi(x,t) = ?$$

Assuming V=V(x), we can solve it via separation of variables:

1) Solve time-indep. S eq $\Rightarrow$ infinite set of slns. $\{\psi_n(x)\}$
$\{E_n\}$

2) To fit $\Psi(x,0)$, linear combination:

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

You can always match the initial state choosing $\{c_n\}$.

Structure of a typical QM problem

3) To construct $\Psi(x,t)$, you add the wiggle factor.

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_n}{\hbar}t} = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)}$$

4) The separable slns are stationary states.

$$\Psi_n(x,t) = \psi_n(x)\, e^{-\frac{iE_n t}{\hbar}}$$

- All prob. and expectation values are independent of t.
- Property not shared by the general solution

↳ energies are different for different ψ_n, so "e" do not cancel out.

Structure of a typical QM problem

What is the physical meaning of $\{c_n\}$?

$|c_n|^2$ is the prob. that a measurement of the energy return E_n.

* Measurement yields one allowed value.

$$\Rightarrow \boxed{\sum_{n=1}^{\infty} |c_n|^2 = 1}$$

$$\Rightarrow \boxed{\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n}$$ Expectation value of the energy.

* $\{c_n\}$ do not depend on time.

$\Rightarrow \langle H \rangle$ do not " " " $\Rightarrow$ energy conservation in QM.

1) Null potential: free QM particles

For a free particle: $V(x) = 0$, there are no boundary conditions

Sch. eq of a free particle:

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

A possible sln was: $\Psi = e^{ikx - i\omega t}$

$$E = \frac{p^2}{2m} = \frac{(\hbar^2 k^2)}{2m}$$

In a general way: $\Psi = \psi(x)\varphi(t)$

$$E = \cancel{\hbar}\omega = \frac{\hbar^{\cancel{2}} k^2}{2m}$$

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

Sch eq. $\Longrightarrow$

$$\begin{cases} i\hbar \dfrac{1}{\varphi}\dfrac{d\varphi}{dt} = E \\[2ex] -\dfrac{\hbar^2}{2m}\dfrac{1}{\psi}\dfrac{d^2\psi}{dx^2} + \cancelto{0}{V} = E \end{cases} \Rightarrow \boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi}$$

time-independent Sch eq

1) Null potential: free QM particles

$\Rightarrow \dfrac{d^2\psi}{dx^2} = -k^2\psi$; where $k = \dfrac{\sqrt{2mE}}{\hbar}$

sln

$\Rightarrow \boxed{\psi(x) = Ae^{ikx} + Be^{-ikx}}$ General sln. for x.

↳ the particle can carry any (positive) energy.

$$\Rightarrow \Psi(x,t) = Ae^{ikx - i\frac{\hbar k^2}{2m}t} + Be^{-ikx - i\frac{\hbar k^2}{2m}t}$$

$$\Psi(x,t) = Ae^{ik[x - \frac{\hbar k}{2m}t]} + Be^{-ik[x + \frac{\hbar k}{2m}t]}$$

$$\boxed{\Psi(x,t) = Ae^{ik(x - vt)} + Be^{-ik(x + vt)}}$$

$\rightarrow$ $\leftarrow$

This term $(x \mp vt)$ implies we have a wave of unchanging shape going in the $\pm x$ direction.

$(x \mp vt) = \text{constant} \Rightarrow x = \text{constant} \pm vt$

1) Null potential: free QM particles

$$\Rightarrow \boxed{\Psi_k(x,t) = A\, e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)}}$$

$$k \equiv \pm \frac{\sqrt{2mE}}{\hbar} \quad \begin{cases} k>0 & \text{wave} \rightarrow \\ k<0 & \text{wave} \leftarrow \end{cases}$$

The stationary states of the free particle are propagating waves, with $\boxed{\lambda = \frac{2\pi}{|k|}}$, momentum $\boxed{p = \hbar k}$, and speed:

$$v_{quantum} = \frac{\hbar |k|}{2m} = \sqrt{\frac{E}{2m}}\,.$$

But, there are two problems.

1) Null potential: issues with plane wave solutions

1) The classical speed of a free particle with $E = \frac{1}{2} m v^2$ is

$$v_{classical} = \sqrt{\frac{2E}{m}} = 2\, v_{quantum}.$$

* The QM wave travels at $\frac{1}{2}\, v_{particle}$?! (Paradox)

2) This wave function is not normalisable.

$$\int_{-\infty}^{+\infty} \Psi_k^* \Psi_k \, dx = \int_{-\infty}^{+\infty} |A|^2 e^{i\alpha} e^{-i\alpha} dx = |A|^2 \int_{-\infty}^{+\infty} dx$$

$$= |A|^2 \, x \Big|_{-\infty}^{+\infty} = |A|^2 (\infty) \quad \text{(Big problem)}$$

* Sep. sln do not represent physical states!
* A free particle cannot exist in a stationary state!
* A free particle with definite E cannot exist!

1) Null potential: free QM particles

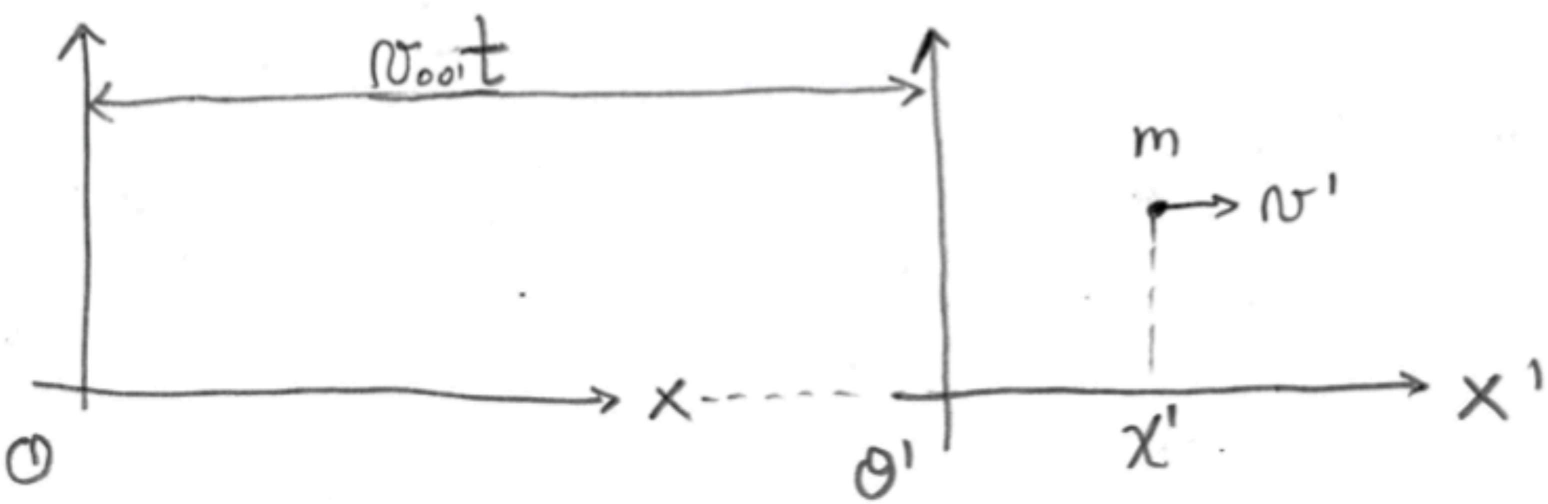
Problem 1: Quantum waves are <u>NOT</u> ordinary (classical) waves.

de Broglie: $\lambda = \dfrac{h}{p}$.

$\psi(x,t) \in \mathbb{C}$ $\begin{cases} \text{Is it measurable?} \\ \text{What's its meaning?} \end{cases}$

Imagine we have 2 observers who measure $\binom{\lambda}{p}$ moving at constant speeds with respect to each other, do their measurements agree?

$$p = \frac{h}{\lambda} = \left(\frac{h}{2\pi}\right)\left(\frac{2\pi}{\lambda}\right) = \hbar \underbrace{k}_{\text{wave number}}$$



$\begin{cases} \text{velocity: } v,\ v' \\ \text{momentum: } p,\ p' \end{cases}$

1) Null potential: free QM particles

$$\left.\begin{aligned} x' &= x - v_{00'}t \\ t' &= t \end{aligned}\right\} \text{Galilean transformation}$$

$$\frac{dx'}{dt'} = \frac{dx}{dt} - v_{00'} \Rightarrow v' = v - v_{00'}$$

$$\Rightarrow p' = p - m v_{00'}$$

In the lab:

de Broglie λ do not agree.

$$\lambda = \frac{h}{p} \qquad \lambda' = \frac{h}{p'} = \frac{h}{p - m v_{00'}} \Rightarrow \boxed{\lambda \neq \lambda'}$$

For ordinary waves, this does NOT happen. λ does not change.

Phase of the wave: $\phi = kx - \omega t$

ϕ is a Galilean invariant, 2 obs. will agree on the value of the phase.

$$\Rightarrow \phi = k\left(x - \frac{\omega}{k}t\right) = \frac{2\pi}{\lambda}(x - Vt)$$

↳ velocity of the wave.

$$\phi = \overset{k}{\frac{2\pi x}{\lambda}} - \overset{\omega}{\frac{2\pi V}{\lambda}}\, t$$

1) Null potential: free QM particles

O' should see the same phase: $\phi' = \phi$ (same point, same t)

$$\phi' = \phi = \frac{2\pi}{\lambda}(x - Vt)$$

$$= \frac{2\pi}{\lambda}(x' + vt - Vt)$$

$$= \frac{2\pi}{\lambda}(x' + vt' - Vt') = \overbrace{\frac{2\pi}{\lambda}}^{k'} x' - \overbrace{\frac{2\pi V}{\lambda}\left(1 - \frac{v}{V}\right)}^{\omega'} t'$$

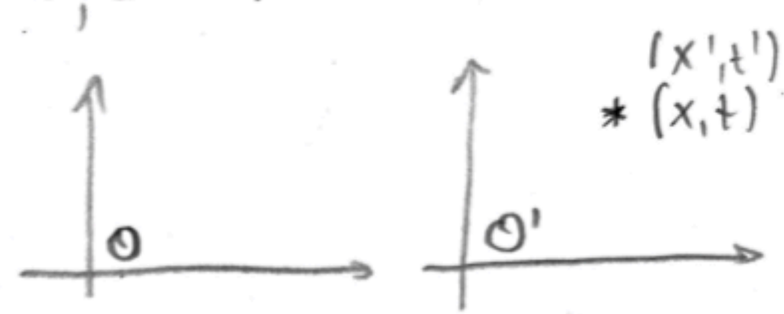
$$\Rightarrow \begin{cases} \omega' = \omega\left(1 - \frac{v}{V}\right) \\ k' = k \;\Rightarrow\; \frac{2\pi}{\lambda'} = \frac{2\pi}{\lambda} \;\Rightarrow\; \boxed{\lambda' = \lambda} \end{cases}$$ for ordinary waves.

$\Rightarrow$ QM waves are not ordinary waves.

$\Rightarrow$ 2 obs. would not agree on the value of the wavefunction Ψ.

$\Rightarrow$ Ψ is not directly measurable, but measurements can still be compared.

$\Rightarrow$ Ψ is not Galilean invariant.



$$\boxed{\Psi \neq \Psi'}$$

1) Null potential: free QM particles

Frequency of matter waves:

$p = \hbar k$

$E = \hbar \omega \Rightarrow \omega = \frac{E}{\hbar}$

Wave phase: $\phi = kx - \omega t$

phase velocity: $v_{phase} = \frac{\omega}{k} = \frac{E}{p} = \frac{\frac{1}{2}mv^2}{mv} = \frac{1}{2}v$.

$$\Rightarrow \boxed{v_{phase} = \frac{1}{2}v}$$ Same result!

- If the plane wave carries no real information, it is not a signal.
- Representing travelling information with plane waves is wrong,
- We need wave packets.
- Phase velocity is not meaningful physically.

1) Null potential: free QM particles

- We can use the group velocity.

$$v_{group} = \left.\frac{d\omega}{dk}\right|_{k_0} = \frac{dE}{dp} = \frac{d}{dp}\left(\frac{p^2}{2m}\right) = \frac{p}{m} = v$$

↑ value of k at which propagation occurs.

⇒ the v_{group} of a wave packet is the velocity of the particle.

Problem 2:

<u>Wave packets</u>

Can be constructed from the superposition of waves.

Remember: $\Psi_k(x,t) = A e^{i\underbrace{\left(kx - \frac{\hbar k^2}{2m}t\right)}_{\phi \equiv \text{phase of the wave}}}$; $\omega(k) = \frac{\hbar k^2}{2m}$

Superposition:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$$

1) Null potential: wave packets

Wave packet:

k continuous

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}\, dk}$$

↗ each state can have a different amplitude

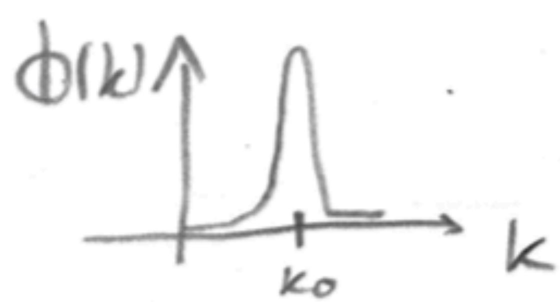
↳ wp is a superposition of sin functions modulated by ϕ

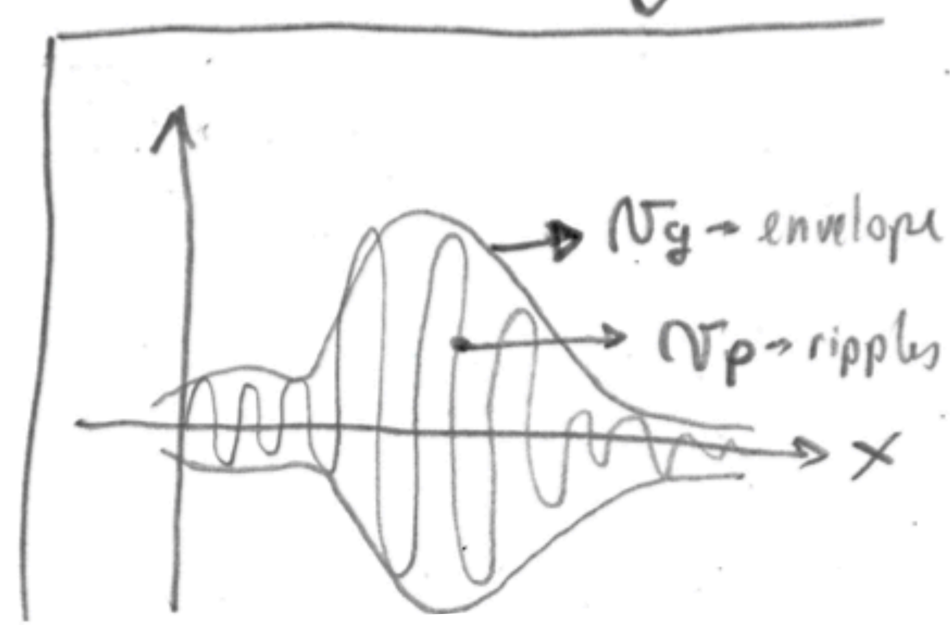
↳ ripples contained within an envelope (v_g)

1. $C_n \rightsquigarrow \frac{1}{\sqrt{2\pi}} \phi(k)\, dk$

2. This can be normalised for an appropriate $\phi(k)$ and

   $\phi(k)$ should peak:





3. wp. carries a range of k, E, v.

1) Null potential: wave packets

How do wave packets move?

Principle of stationary phase $(kx - \omega(k)t)$

At $k \approx k_0$ the $\int$(function x wave) can be non-zero

$\phi = kx - \omega t \rightarrow$ phase should be stationary wrt k at k_0 ↱ constant

$$\left.\frac{d\phi}{dk}\right|_{k_0} = x - \left.\frac{d\omega}{dk}\right|_{k_0} t = 0$$

$$\Rightarrow x = \left.\frac{d\omega}{dk}\right|_{k_0} t \Rightarrow \boxed{x = v_{group}\, t}$$

The shape of the wave moves with v_{group}.

In QM, we are given: $\Psi(x,0)$, and need to find $\Psi(x,t)$

=> we need to find $\phi(k)$ to match $\Psi(x,0)$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, dk$$; $\phi(k)$ is F. transf of $\Psi(x,0)$.

1) Null potential: Plancherel's theorem

We can use Fourier analysis, in particular Plancherel's theorem:

$$\int_{-\infty}^{+\infty} |f(x)|^2 dx = \int_{-\infty}^{+\infty} |F(k)|^2 dk$$

$$\int_{-\infty}^{+\infty} f(x)\, g^*(x)\, dx = \int_{-\infty}^{+\infty} F(k)\, G^*(k)\, dk$$

$$\downarrow$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, dk$$

$$\Leftrightarrow \boxed{\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0)\, e^{-ikx}\, dx}$$

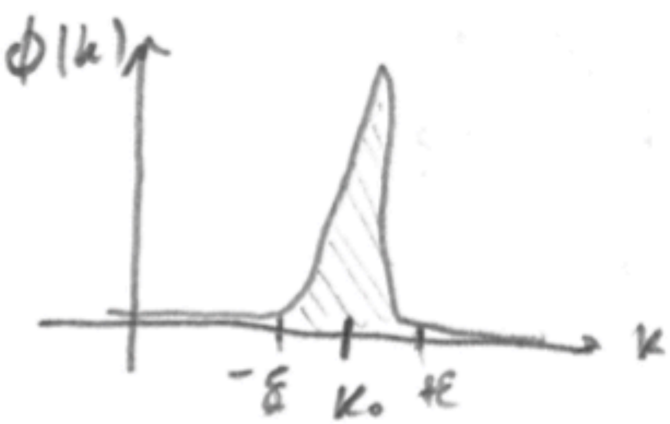
1) Null potential: Phase and Group Velocities

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i(kx-\omega t)}\, dk$$

with $\omega = \frac{\hbar k^2}{2m}$, which is called the dispersion relation of the wp.

$\phi(k)$ is narrowly peaked at k_0,

$\Rightarrow$ we can taylor-expand $\omega(k)\big|_{k_0}$



$$\omega(k) = \omega(k_0) + (k-k_0)\frac{d\omega}{dk}\Big|_{k_0} + \cancelto{0}{\mathcal{O}\left((k-k_0)^2\right)}$$ $\rightsquigarrow$ distorsion of wave pattern.

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, e^{-i\omega_0 t}\, e^{-ik\omega_0' t}\, e^{+ik_0\omega_0' t}\, dk$$

1) Null potential: Phase and Group Velocities

①

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \underbrace{e^{-i\omega_0 t} e^{+ik_0\omega_0' t}}_{\text{pure phase}} \underbrace{\int_{-\infty}^{+\infty} \phi(k) e^{ik(x-\omega_0' t)} dk}_{\text{Similar to:}}$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} dk$$

$$\Rightarrow \boxed{|\Psi(x,t)| = |\Psi(x-\omega_0' t, 0)|}$$

② $s \equiv k - k_0$

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i(s+k_0)x}\, e^{-i(\omega_0 t + (k_0+s)\omega_0' t - ik_0\omega_0' t)} ds$$

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i[(s+k_0)x - (\omega_0 + \omega_0' s t)} ds$$

1) Null potential: Phase and Group Velocities

Then: $$\Psi(x,t) = \underbrace{\frac{1}{\sqrt{2\pi}} e^{i(k_0 x - \omega_0 t)}}_{\substack{\text{sinusoidal wave} \\ \text{"ripples"}}} \underbrace{\int_{-\infty}^{\infty} \phi(k_0+s)\, e^{is(x-\omega_0' t)}\, ds}_{\text{envelope}}$$

$$\frac{\omega_0}{k_0} \qquad\qquad \omega_0'$$

Phase velocity:

$$v_{phase} = \left.\frac{\omega}{k}\right|_{k_0}$$

Group velocity

$$v_{group} = \left.\frac{d\omega}{dk}\right|_{k_0}$$

1) Null potential: Phase and Group Velocities

In our case:

$$\omega(k) = \frac{\hbar k^2}{2m} \Rightarrow \frac{d\omega}{dk} = \frac{\hbar k}{m}$$

$$\Rightarrow \boxed{v_{group} = v_{classical} = 2\, v_{phase}}$$

$$v_{group} = \frac{dE}{dt} = \frac{d}{dt}\left(\frac{p^2}{2m}\right) = \frac{p}{m} = v_{classical} \checkmark$$

Notes:

1) ψ cannot be $\mathbb{R}$.

2) Sch. eq is not a wave equation of the classical type:

$$\frac{\partial^2 y}{\partial t^2} = v^2 \frac{\partial^2 y}{\partial x^2} \Rightarrow \boxed{y = f(x - vt) + g(x + vt)} \in \mathbb{R}$$

Example: $\boxed{y(x,t) = A \sin(x - vt) + B \sin(x + vt)}$

Canonical commutation relation

The $\hat{x}$ operator

$$\text{Sch. eq: } \underbrace{i\hbar\frac{\partial}{\partial t}}_{\text{operator}}\Psi = \overbrace{\left(\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\text{operator}} + \underbrace{V}_{\text{operator} \to V(x,t)}\right)}^{\hat{H} \equiv \text{Hamiltonian}}\Psi$$

We can introduce an operator $\hat{x}$, which is a multiplication operator. When applied on a function of x, it multiplies it by x.

$$\Rightarrow \hat{x}\cdot F(x) = x\cdot F(x)$$

In QM, we have a few operators: $\hat{x}$, $\hat{p}$, $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x},t)$

Operators are matrices, so the order in which we multiply them makes a difference. Does the order matter when multiplying $\hat{x}$ and $\hat{p}$? (Heisenberg)

$$(\hat{x}\hat{p} - \hat{p}\hat{x})\Psi = 0 \;?? \quad \Rightarrow \hat{x}\hat{p}\Psi - \hat{p}\hat{x}\Psi = ? \quad ; \; \Psi(x,t)$$

Canonical commutation relation

$$\hat{x}(\hat{p}\psi) - \hat{p}(\hat{x}\psi) = \hat{x}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\right) - \hat{p}(x\psi)$$

$$= \frac{\hbar}{i} x \frac{\partial\psi}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}(x\psi)$$

$$= \frac{\hbar}{i} x \frac{\partial\psi}{\partial x} - \frac{\hbar}{i} x \frac{\partial\psi}{\partial x} - \frac{\hbar}{i}\psi = -\frac{\hbar}{i}\psi = i\hbar\psi$$

$$\Rightarrow (\hat{x}\hat{p} - \hat{p}\hat{x})\psi = i\hbar\psi$$

$$\Rightarrow \boxed{(\hat{x}\hat{p} - \hat{p}\hat{x}) = i\hbar}$$ equality between operators.

This is called a commutator: $[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$

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

Canonical commutation relation.

Operators : wavefunctions, eigenstates

Matrices : vectors , eigenvectors