6.6 Application to free particle moving along a line

6.6.1. Schrödinger Equation for a free particle

A particle of mass m that can move freely along a line is described by the Hamilton Operator

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

in direct analogy of the energy of a classical particle, which has kinetic energy $\frac{1}{2}mv^2$

So the Schrödinger Equation is

(abstract bra-ket notation)

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \frac{\hat{p}^2}{2m}|\psi(t)\rangle$$

in (position-coordinate representation)

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

Schrödinger Equation for a free particle on a line

Note: now writing partial derivatives, as we have now two variables: x and t

6.5.2 Solving Strategy:

In the discrete cases, we just looked for

- characteristic polynomial of H ==> eigenvalues λ_i
- for each eigenvalue, search for eigenvector

$$H|\lambda_i\rangle = \lambda_i|\lambda_i\rangle$$

In the continuous case, we don't have the tool of the characteristic polynomial at our hand!

==> need individual strategies to find eigenvectors and eigenvalues

==> physics/math built up a toolbox for these problems

With known Eigenvectors and eigenvalues the time evolution of an initial state can be easily performed, in close analogy what has been done in the case of finite dimensional vector space:

Time Evolution: Coordinate representation in Energy Eigenbasis (time independent Hamiltonian)

Schrödinger Equation

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

expansion in eigenstates of H:

$$|\Psi(t)\rangle = \sum_n c_n(t)|E_n\rangle$$

dynamical equation: $i\hbar\frac{d}{dt}c_n(t) = E_n c_n(t)$

initial values: $c_n(0) = c_n$

➔ $c_n(t) = c_n\, e^{-i\frac{E_n t}{\hbar}}$

Solution of Schrödinger's equation via Energy Eigenstates:

Step 1: find eigenvectors $|E_n\rangle$ and eigenvalue E_n of H

Step 2: Expand initial state in eigenbasis

$$|\Psi(0)\rangle = \sum_n c_n|E_n\rangle$$

Step 3: Write down solution

$$|\Psi(t)\rangle = \sum_n c_n\, e^{-i\frac{E_n t}{\hbar}}|E_n\rangle$$

6.6.2 Eigenstates and eigenvalues of Hamiltonian

Momentum states $|p\rangle$ are eigenstates of the Hamiltonian with eigenvalues

$$E = \frac{p^2}{2m}$$

$\Rightarrow$ **degenerate** eigenspaces:

$$E = \frac{p^2}{2m} \iff \left\{ \begin{matrix} |+p\rangle \\ |-p\rangle \end{matrix} \right. \quad p = \pm\sqrt{2mE}$$

let us introduce as abbreviation

wave number $\quad k = \frac{\sqrt{2mE}}{\hbar} \Rightarrow p = \pm k\hbar$

connection wave number to wave length: $k = \frac{2\pi}{\lambda}$

so a general eigenstate to the Hamiltonian Operator of a free particle with energy E can be written as

$$|\psi_E\rangle = \alpha|+p\rangle + \beta|-p\rangle$$

$$\Rightarrow \psi_E(x) = \frac{1}{\sqrt{2\pi\hbar}}\left(\alpha \underbrace{e^{ikx}}_{\langle x|p\rangle} + \beta \underbrace{e^{-ikx}}_{\langle x|-p\rangle}\right)$$

coordinate representation

Because of the degeneracy of the energy eigenvalues, we will use always the momentum p to characterize the eigenstates, rather than the eigenenergy E:

energy eigenstates

eigenvalue E, degenerate eigenstates (two eigenstates per eigenvalue)

$E \in [0, \infty)$ $\quad |p\rangle$ with $p = \pm\sqrt{2mE}$

degenerate

momentum eigenstates:

characterized by momentum p

$p \in (-\infty, +\infty)$ $\quad E = \frac{p^2}{2m}$

6.6.3 Time evolution of Energy Eigenstates

$$e^{-i\frac{Et}{\hbar}}$$

$$|\psi_E(t)\rangle = \alpha e^{-i\frac{p^2}{2m\hbar}t}|p\rangle + \beta e^{-i\frac{p^2}{2m\hbar}t}|-p\rangle$$

$$\Rightarrow \quad \psi_E(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\alpha e^{-i\frac{p^2}{2m\hbar}t} e^{ikx} + \frac{1}{\sqrt{2\pi\hbar}}\beta e^{-i\frac{p^2}{2m\hbar}t} e^{-ikx}$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\left(\alpha e^{-i(\omega t - kx)} + \beta e^{-i(\omega t + kx)}\right)$$

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

$$k = \frac{\sqrt{2mE}}{\hbar} = \frac{p}{\hbar}$$

Solutions are moving waves: (de Broglie Relationship)

$e^{-i(\omega t + kx)}$; left moving wave with angular frequency $\omega = 2\pi\nu$ wave number k

$e^{-i(\omega t - kx)}$ right moving wave with angular frequency ω wave number k

We used these waves for our Davisson-Germer Experiments!

phase velocity

$$V_{ph} = \nu\lambda = \frac{\omega}{k} = \frac{p^2 \hbar}{2m\hbar\, p} = \frac{p}{2m} = \frac{V_{classical}}{2}$$

experience with waves (light) tells us that the phase velocity is not what counts as propagation speed of a wavepacket (pulse). That velocity is typically characterized by the group velociy?

group velocity: $$V_{group} = \left.\frac{d\omega}{dk}\right|_{k_0} = \frac{d}{dk}\left(\frac{k^2\hbar}{2m}\right) = \frac{2k\hbar}{2m} = \frac{2p}{2m} = \frac{p}{m} = V_{classical}$$

6.6.4 Time evolution for general initial state

The most general solution is then given by writing the initial state as a linear combination of momentum eigenstates (all integrals from $-\infty$ to $+\infty$)

$$|\psi(0)\rangle = \int dp\, |p\rangle\langle p|\psi(0)\rangle$$

$$= \int dp\, \psi_p(p,0)\, |p\rangle$$

Note: as state before, we parameterize the eigenstates by p, not by E! - this is more convenient due to the degeneracy of the eigenspaces

$$\psi_p(p,0) = \langle p|\psi(0)\rangle$$

$$= \int dx\, \langle p|x\rangle\langle x|\psi(0)\rangle$$

$$= \int dx\, \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{px}{\hbar}}\, \psi(x,0)$$

(complex Fourier transform of initial wave function!)

Then we have for the general solution at some later time

$$|\psi(t)\rangle = \int dp\, \psi_p(p,0)\, e^{-i\frac{p^2}{2m}\frac{t}{\hbar}}\, |p\rangle \qquad = e^{-i\frac{Et}{\hbar}} \qquad E = E(p)$$

Going back to the coordinate representation with respect to the position, we find

$$\langle x|\psi(t)\rangle = \int dp\, \psi_p(p,0)\, e^{-i\frac{p^2}{2m}\frac{t}{\hbar}}\, \langle x|p\rangle$$

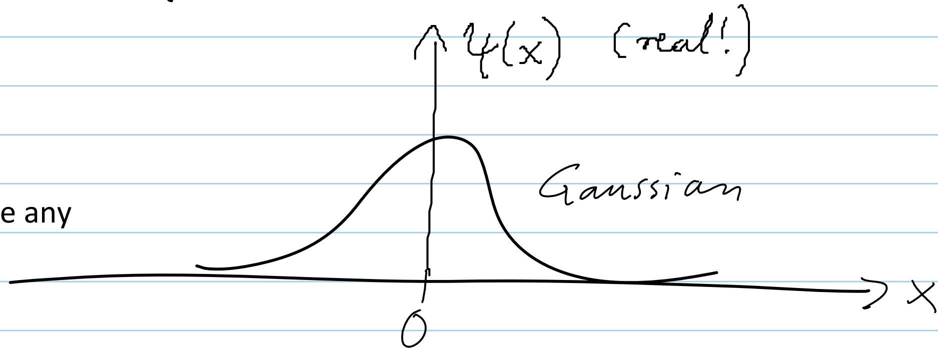
$$\psi(x,t) = \int dp\, \psi_p(p,0)\, e^{-i\frac{p^2 t}{2m\hbar}}\, \frac{1}{\sqrt{2\pi\hbar}}\, e^{i\frac{px}{\hbar}}$$

6.6.5 Example Spreading of wave function (simulation)

initial state

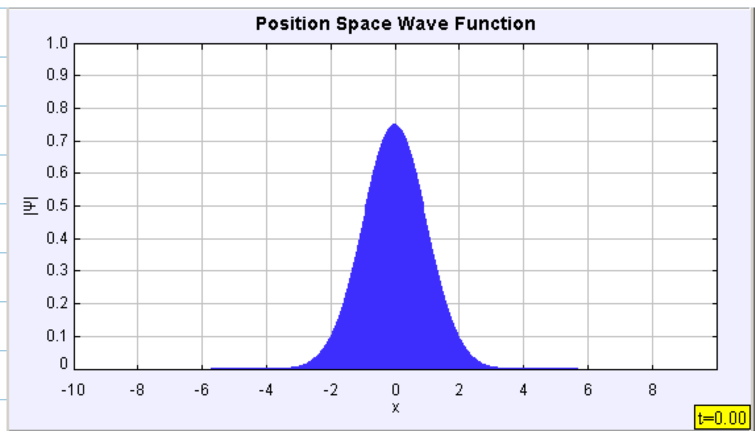
$$\psi(x) = \frac{1}{(2\pi)^{1/4}} \frac{1}{\sqrt{\Delta \hat{x}}} e^{-\left(\frac{1}{2}\frac{x}{\Delta \hat{x}}\right)^2}$$

(We omit here any derivation)



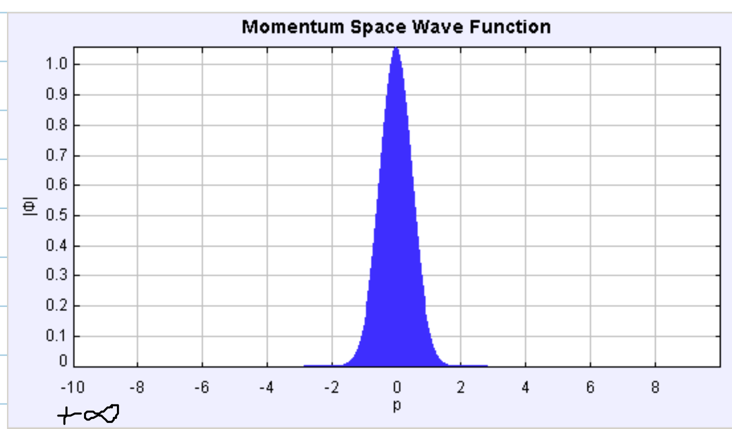
As can be seen from simulations, a particle described initially by a Gaussian wave packets (minimum uncertainty state) will get wider and wider ...
Interpretation: The more you confine the initial wave-packet to a narrow region, the higher must be the variance of momentum
==> particle will not be at rest, but move away from initial position
==> spreading

Initial state: $\psi(x,0)$



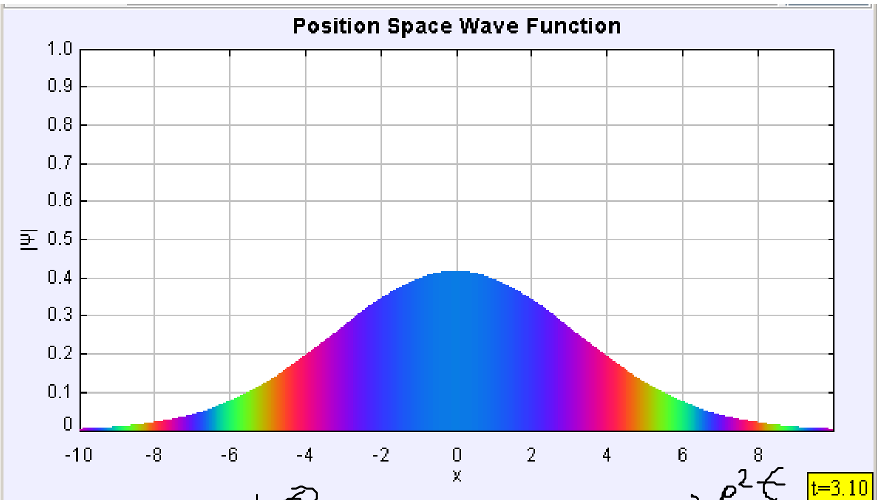
This gives

$\psi_p(p,0)$



$$\psi_p(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx\, e^{-i\frac{px}{\hbar}} \psi(x,0)$$

Then at a later time we find



colouring corresponds to complex phase of wavefunction

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

$\Rightarrow$ the wave function spreads out!

6.6.6 Time Evolution and initial values

Classical mechanics:

$$F = ma$$

$$m\ddot{x} = -\frac{d}{dx}V(x)$$

free particle: $V(x) = 0$

initial values:

initial position x(t)

initial velocity $\dot{x}(0) \equiv \frac{d}{dt}x(t)\Big|_{t=0}$

Quantum Mechanics:

Initial value:

$\psi(x,0)$ (leading to $\psi_p(p,0)$)

Only initial position fixed?

NO! $\psi(x,0)$ $\Rightarrow |\langle x|\psi(0)\rangle|^2 dx = |\psi(x,0)|^2 dx$

initial position (distribution)

$\Rightarrow |\langle p|\psi(0)\rangle|^2 dp = |\psi_p(p,0)|^2 dp$

initial momentum (distribution)

Initial spatial distribution fixes

$$|\psi(x,0)|^2$$

so we can write all initial states with the same initial spatial distribution as

$$\psi(x,0) = |\psi(x,0)| \, e^{i f(x)}$$

$$f(x) \in \mathbb{R}$$

so the information about the initial momentum distribution sits in the complex phase $e^{i f(x)}$ of the initial wave function $\psi(x,0)$!