Quantum Communications

Lecture notes

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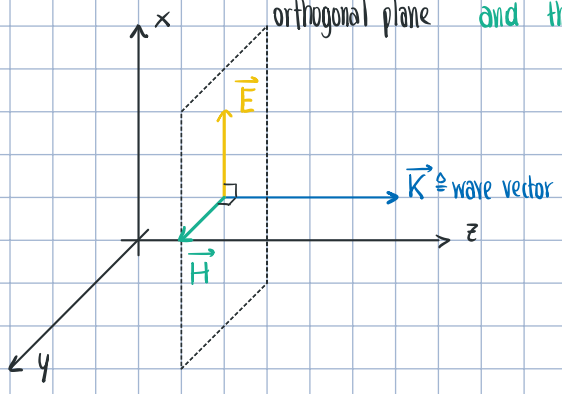
CLASSICAL OPTICS

Optics is a branch of electromagnetism and the light is described as an electromagnetic wave.

An ideal solution of the Maxwell's equation is the plain monochromatic wave, but this solution has some issues ⟶ infinite amount of energy.

monochromatic → single-frequency spectrum: ν [Hz]
(angular frequency or pulsation $\triangleq \omega = 2\pi\nu$ [rad s^{-1}])

plain → the phase is constant over any plane orthogonal to the propagation direction and the amplitude is constant everytime.



We can say that this plain wave is a TEM wave (Transverse Electric and Magnetic wave).

- $|\vec{K}| = \frac{2\pi}{\lambda}$ ⟶ wavelength $= \frac{\text{phase variation}}{\text{length variation}}$
- $\vec{K}$ is always parallel to the propagation direction
- $\vec{E}, \vec{H}, \vec{K}$ form a set of a three mutually orthogonal

The electric field for this solution depends only on z and time:

$$E_x(z,t) = A_x \cdot \cos(\text{phase term}) = A_x \cdot \cos(Kz - \omega t + \delta_x)$$

A_x → amplitude; δ_x → phase offset (constant)

Kz → plane wave directed to the positive z

$\Delta z = \frac{\omega}{K}\Delta t \Rightarrow$ velocity of the wave: $v = \nu\lambda$

In vacuum, the velocity of the electromagnetic wave is

$$v_0 = \lambda_0 \nu = c = 299792458 \text{ m/s} \simeq 3 \cdot 10^8 \text{ m/s}$$

In a homogeneous and isotropic medium (e.g. air, water, glass) we can define the index of refraction:

$$\boxed{v = \frac{c}{n}} \leq c \quad \text{because} \quad n \geq 1 \quad (n=0 \text{ in vacuum}).$$

→ the frequency does not vary from medium to medium: $\boxed{\lambda = \frac{\lambda_0}{n}}$

For the y and z direction, the electric field can be written as

$$E_y(z,t) = A_y \cos(Kz - \omega t + \delta_y)$$

$$E_z(z,t) = 0$$

The dimensionality of light is 2 ⟶ the plane wave is described by two scalar components

The Maxwell's equations are linear partial differential equations in $\vec{E}$ and $\vec{H}$ so we can apply the superposition of effects and represent the electric and magnetic field with the complex representation:

$$\tilde{E}_x(z,t) = A_x e^{i(kz-\omega t+\delta_x)} = A_x e^{ikz} e^{-i\omega t} e^{i\delta_x} = \underbrace{\left[A_x e^{i\delta_x}\right]}_{\text{constant complex number (phasor)}} e^{ikz} e^{-i\omega t}$$

$$E_x(z,t) = \mathrm{Re}\left\{\tilde{E}_x(z,t)\right\}$$

$$\left[= \mathrm{Re}\left\{A_x\left[\cos(kz-\omega t+\delta_x) + i\sin(kz-\omega t+\delta_x)\right]\right\} = A_x\cdot\cos(kz-\omega t+\delta_x)\right]$$

$$\tilde{E}_x(z,t) = \left(A_x e^{i\delta_x}\right) e^{ikz} e^{-i\omega t} = \tilde{E}_{ox} e^{ikz} e^{-i\omega t}$$

$$\tilde{E}_y(z,t) = \left(A_y e^{i\delta_y}\right) e^{ikz} e^{-i\omega t} = \tilde{E}_{oy} e^{ikz} e^{-i\omega t}$$

$$\downarrow$$

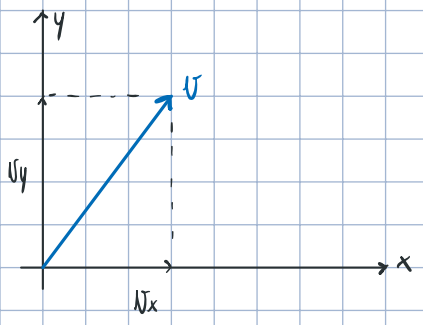
$$\tilde{E}(z,t) = \underbrace{\begin{bmatrix}\tilde{E}_{ox}\\ \tilde{E}_{oy}\end{bmatrix}}_{\text{JONES VECTOR}} e^{ikz} e^{-i\omega t}$$

JONES VECTOR: represent the state of polarization of the electromagnetic wave

The state of polarization of light is described by the Jones vector (is a vector with two complex component ⇒ it's an element of a complex 2-D vectorial space)

2-D HILBERT SPACE

To make an analogy: in euclidean geometry (of the plane, for instance) a vector could be completely described by a pair of components, the x and the y component.



$\begin{bmatrix}v_x\\ v_y\end{bmatrix}$ is a element of 2D euclidean vectorial spaces.

For the state of polarization of light, the Jones vectors are elements of 2D Hilbert space.

In the Hilbert space we can also define the scalar product between two Jones vectors:

$$\begin{bmatrix}u_x\\ u_y\end{bmatrix} \text{ and } \begin{bmatrix}v_x\\ v_y\end{bmatrix} \xrightarrow{\text{scalar prod.}} \begin{bmatrix}u_x\\ u_y\end{bmatrix}^{\dagger}\cdot\begin{bmatrix}v_x\\ v_y\end{bmatrix} = \underbrace{\begin{bmatrix}u_x^* & u_y^*\end{bmatrix}}_{\text{matrix (1,2)}}\cdot\underbrace{\begin{bmatrix}v_x\\ v_y\end{bmatrix}}_{\text{matrix (2,1)}} = \underbrace{u_x^* v_x + u_y^* v_y}_{\text{matrix (1,1) = scalar}}$$

dagger operation

The dagger operation for complex matrix is simply the conjugated transposition operation.

Two (non-zero) Jones vectors are <u>equivalent</u> if and only if one vector is the product of the other vector by a complex scalar coefficient. This is important because two states of polarization (and later qubit) are identical if the two Jones vectors are equivalent.

The states of polarization are equivalence classes in the Hilbert space of Jones vector, said rays (according to the previous definition of equivalence). For analogy with the euclidean geometry:

$$\begin{bmatrix} v_x \\ v_y \end{bmatrix} \text{ is equivalent to } a\begin{bmatrix} v_x \\ v_y \end{bmatrix} = \begin{bmatrix} a\,v_x \\ a\,v_y \end{bmatrix}, \text{ for any real } a \neq 0.$$

We consider a

$$\vec{\tilde{E}}(z,t) = \begin{bmatrix} \tilde{E}_{0x} \\ \tilde{E}_{0y} \end{bmatrix} e^{ikz} \cdot e^{-i\omega t}$$

Jones vector

The Jones vector gives the polarization of the wave.

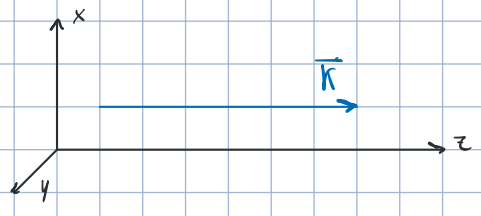
$$\begin{cases} \tilde{E}_{0x} = A_x e^{i\delta_x} \\ \tilde{E}_{0y} = A_y e^{i\delta_y} \end{cases}$$

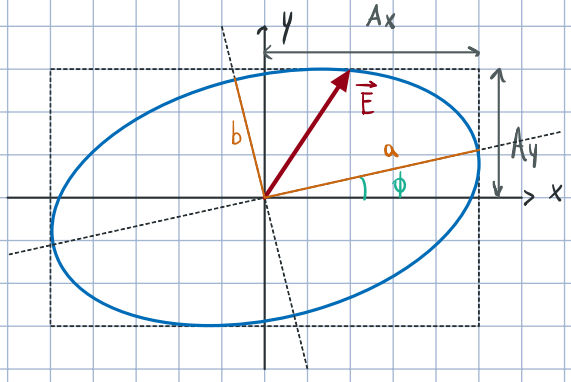
To characterize the state of polarization there are some parameters:

A_y / A_x

$\delta = \delta_y - \delta_x$

By looking the plane where both the x-electric field and y-electric field lay, we can see that the overall electric field vector describes an ellipse, called ELLIPSE OF POLARIZATION.





The period is defined as $T = 1/\nu$

The electric field vector rotates correspondgly

- anti-clockwise moment of $\vec{E}$ (positive handedness) ⟶ left elliptical states of polarization
- clockwise moment of $\vec{E}$ ⟶ right elliptical states of polarization

Other parameters to describe the ellipse of polarization are:

- $\phi \triangleq$ azimuth: orientation angle of the major axis (with respect to x axis)
- $\chi \triangleq$ ellipticity: ⟶ $+ \arctan(b/a)$ for left states; ⟶ $- \arctan(b/a)$ for right states

$$-\pi/4 \leq \chi \leq \pi/4$$

where $\begin{cases} a = \text{major semi-axis length} \\ b = \text{minor semi-axis length} \end{cases}$

LINEAR STATES OF POLARIZATION

Are a particular case where the elipse collapses to a segment. This condition is met when $b = 0$.

Then:

$\phi \triangleq$ angle of the axis of oscillation of $\vec{E}$

$\chi = \arctan(b/a) = \arctan(0) = 0$

It is no more possible to see a sense of rotation of the electric field vector.

CIRCULAR STATES OF POLARIZATION

In this case instead the ellipse collapses to a perfect circle, so when $a = b$. In this case the sense is still visible, so:

- left circular state: $\chi = +\arctan(1) = +\pi/4$
- right circular state: $\chi = -\arctan(1) = -\pi/4$

However, since we can not distinguish anymore the major and the minor semi-axis, the azimuth ϕ is indefinite.

We can also define the <u>NORM of a vector</u> (in a Hilber space):

$\|\cdot\|^2 \triangleq$ the scalar product of the vector with itself

e.g. norm of the Jones vector $\begin{bmatrix} \tilde{E}_{ox} \\ \tilde{E}_{oy} \end{bmatrix}$.

$$\left\| \begin{bmatrix} \tilde{E}_{ox} \\ \tilde{E}_{oy} \end{bmatrix} \right\|^2 = \begin{bmatrix} \tilde{E}_{ox} \\ \tilde{E}_{oy} \end{bmatrix}^{\dagger} \cdot \begin{bmatrix} \tilde{E}_{ox} \\ \tilde{E}_{oy} \end{bmatrix} = \begin{bmatrix} \tilde{E}_{ox}^{*} & \tilde{E}_{oy}^{*} \end{bmatrix} \begin{bmatrix} \tilde{E}_{ox} \\ \tilde{E}_{oy} \end{bmatrix} = \tilde{E}_{ox}^{*} \cdot \tilde{E}_{ox} + \tilde{E}_{oy}^{*} \cdot \tilde{E}_{oy} = |\tilde{E}_{ox}|^2 + |\tilde{E}_{oy}|^2$$

So the squared norm of a vector is the sum of the squared modulus of the components.

The normalization condition for $\begin{bmatrix} \tilde{E}_{ox} \\ \tilde{E}_{oy} \end{bmatrix}$ is $|\tilde{E}_{ox}|^2 + |\tilde{E}_{oy}|^2 = 1$.

So it is easy to write the normalized Jones vector for a linear state of polarization.

- <u>Horizontal state</u> (H):

$$\left.\begin{aligned} A_y &= 0 \\ \tilde{E}_{ox} &= A_x e^{i\delta_x} \\ \tilde{E}_{oy} &= A_y e^{i\delta_y} \end{aligned}\right\} \qquad \begin{bmatrix} A_x e^{i\delta_x} \\ 0 \end{bmatrix} = A_x e^{i\delta_x} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

With squared norm:

$$\left| A_x e^{i\delta_x} \right|^2 \cdot \left(|1|^2 + |0|^2 \right) = \boxed{A_x^2}$$

If $A_x = 1$, the Jones vector for H is normalized and putting $\delta_x = 0 \Rightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

- Vertical state (V):

$$\left.\begin{aligned} A_x &= 0 \\ \tilde{E}_{ox} &= A_x e^{i\delta_x} \\ \tilde{E}_{oy} &= A_y e^{i\delta_y} \end{aligned}\right\} \qquad \begin{bmatrix} 0 \\ A_y e^{i\delta_y} \end{bmatrix} = A_y e^{i\delta_y} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

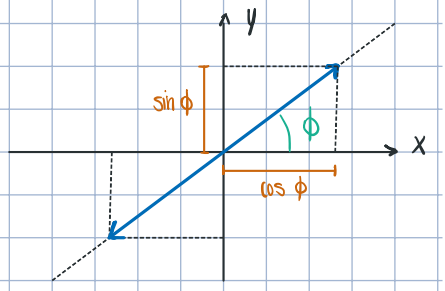
With squared norm:

$$\left| A_y e^{i\delta_y} \right|^2 \cdot \left(|0|^2 + |1|^2 \right) = \boxed{A_y^2}$$

- Linear state ($\chi = 0$) with a generic azimuth ϕ:

$$\begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix} \cdot A e^{i\delta}$$

$$\| \cdot \|^2 = \cos^2\phi + \sin^2\phi = 1$$



- Diagonal (Q) linear state ($\phi = 45°$) and antidiagonal ($-Q$) linear state ($\phi = -45°$):

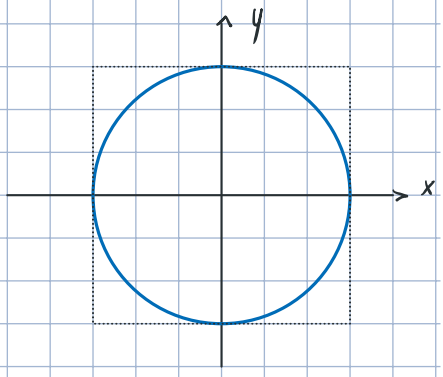
normalized Jones vector for diagonal linear state: $\begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} = 1/\sqrt{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

normalized Jones vector for antidiagonal l.s.: $\begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix} = 1/\sqrt{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

We can verify that the scalar product between Q and $-Q$ is zero $\longrightarrow$ this verifies that this linear states are orthogonal. This is true also for H and V states.

For a circular state instead:

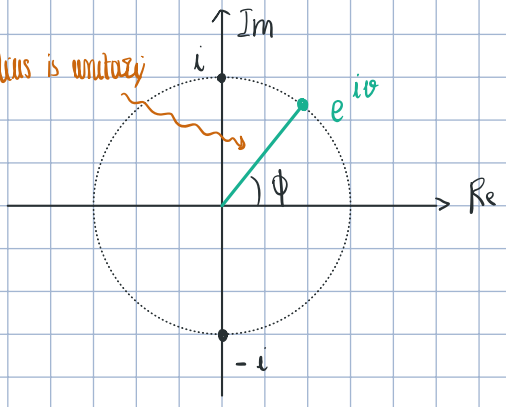
- $A_x = A_y = A$
- $\delta = \delta_x - \delta_y = \pm \pi/2$ (+ for left L, − for right R) ⇝ the two components have to be in quadrature!



The Jones vector for a circular state:

$$\begin{bmatrix} A_x e^{i\delta_x} \\ A_y e^{i\delta_y} \end{bmatrix} = A \begin{bmatrix} e^{i\delta_x} \\ e^{i\delta_y} \end{bmatrix} = A e^{i\delta_x} \begin{bmatrix} 1 \\ e^{i(\delta_x - \delta_y)} \end{bmatrix}$$

$$= A e^{i\delta_x} \begin{bmatrix} 1 \\ e^{\pm i\pi/2} \end{bmatrix} = A e^{i\delta_x} \begin{bmatrix} 1 \\ \pm i \end{bmatrix}$$



For normalization: $A = 1/\sqrt{2}$ and $\delta_x = 0$

$$L: \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} \longrightarrow \|L\|^2 = \left(1/\sqrt{2}\right)^2 \left[|1|^2 + |i|^2 \right] = 1$$

$$R: \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix}$$

The scalar product between L and R:

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}^{+} \cdot \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & -i \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -i \end{bmatrix} = \frac{1}{2} \left[1 \cdot 1 + (-i)(-i) \right] = \frac{1}{2} \left[1 + i^2 \right] = 0$$

They are perfectly orthogonal!

QUASI - TEM monochromatic wave

In case of "smooth" transverse confinement of light.

small direction of the electrical field in a transverse direction for variation of the position in the order of λ

$$\begin{cases} \tilde{E}_x(x,y,z,t) = \Psi_x(x,y,z) \cdot e^{-i\omega t} \\ \tilde{E}_y(x,y,z,t) = \Psi_y(x,y,z) \cdot e^{-i\omega t} \\ \tilde{E}_z(x,y,z,t) \approx 0 \end{cases}$$

Ψ_x, Ψ_y: wave function, they are scalar functions

In case of no polarization coupling: ⟶ during the propagation the Jones vector does not vary

⇒ the polarization remains constant

$$\tilde{E} = \begin{bmatrix} \Psi_x(x,y,z) \\ \Psi_y(x,y,z) \end{bmatrix} e^{-i\omega t}$$

Quasi-TEM monochromatic wave and no polarization coupling:

The last lecture we have found:

$$\begin{bmatrix} \tilde{E}_x \\ \tilde{E}_y \end{bmatrix} = \begin{bmatrix} \text{normalized} \\ \text{Jones} \\ \text{vector} \end{bmatrix} \cdot \Psi(x,y,z)\, e^{-i\omega t}$$

$e^{-i\omega t}$: complex representation of the carrier

$\Psi(x,y,z)$: scalar wave function (complex envelope)

Jones vector: represents the state of polarization

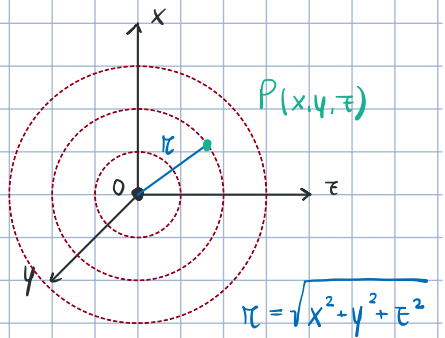
The optical intensity [power over the area – W/m^2] is directly proportional to the squared norm of the complex vector representation:

$$\left\| \begin{bmatrix} \tilde{E}_x \\ \tilde{E}_y \end{bmatrix} \right\|^2 = \left|\tilde{E}_x\right|^2 + \left|\tilde{E}_y\right|^2 = \left|\Psi(x,y,z)\right|^2$$

For a monochromatic plane wave along the z-axis:

$$\Psi(x,y,z) = \underbrace{A_0 e^{i\phi_0}}_{\text{constant vector}} \cdot e^{ikz}$$

For a monochromatic spherical wave diverging from the origin:



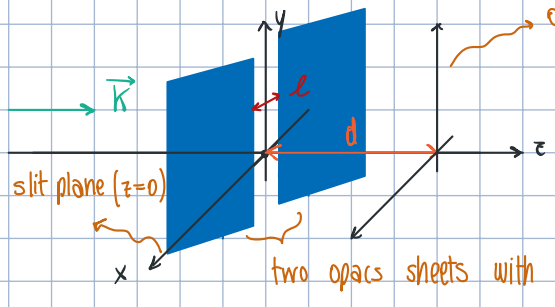
$$\Psi(r) = A_0 e^{i\phi_0} \cdot \frac{e^{ikr}}{r}$$

spherical coordinates

$$\Psi(x,y,z) = A_0 e^{i\phi_0} \cdot \frac{e^{ik\sqrt{x^2+y^2+z^2}}}{\sqrt{x^2+y^2+z^2}}$$

Let's analyze two experiments:

1) DIFFRACTION OF LIGHT BY A SINGLE SLIT

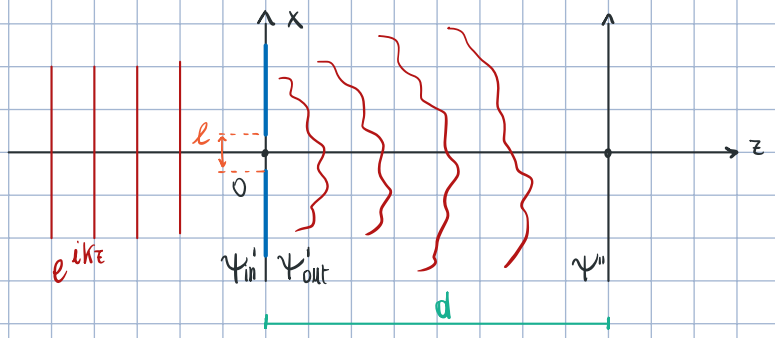


$$\Psi = e^{ikz}$$

$$l \gg \lambda$$

We can use the scalar theory of diffraction (derived from the Huygens principle) to measure the intenisty of the field at a certain distance d.

With the simmetry of the geometry we can view the situation in a 2D plane:



We rename the wave function before entering the slit with ψ'_{in}, with ψ'_{out} the wave function after passing through the slit, and ψ'' the final wave function

$$\psi'_{in} = 1 \cdot e^{ikz}\Big|_{z=0} = e^{ikz}\Big|_{z=0} = 1$$

$$\psi'_{out} = \begin{cases} 1 & \text{for } |x| \leq \ell/2 \\ 0 & \text{elsewhere} \end{cases} \quad \text{or} \quad \psi'_{out} = \text{rect}\left(\frac{x}{\ell}\right) = \begin{cases} 1 & \text{for } -\ell/2 \leq x \leq \ell/2 \\ 0 & \text{elsewhere} \end{cases}$$

We can use the far-field approximation (Fraunhofer diffraction) valid for

$$\frac{(\ell/2)^2}{\lambda d} \ll 1 \quad (\lesssim 0.1)$$

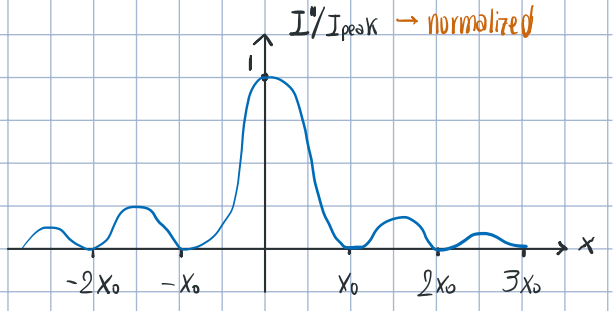
$$\psi'' \propto e^{ikz} \cdot \underline{F}\{\psi'_{out}\} \longrightarrow \psi'' = \frac{\ell}{i\lambda d} e^{ikz} \cdot \text{sinc}\left(\frac{\ell x}{\lambda d}\right)$$

Fourier transform of the rectangle

The first zero of the field at $x_0 = \frac{\lambda d}{\ell}$ while the optical intensity on the observation plane is:

$$I''(x) \propto |\psi''(x)|^2 = \left(\frac{\ell}{\lambda d}\right)^2 \text{sinc}^2\left(\frac{\ell x}{\lambda d}\right)$$

$$I''(x) = I_{peak} \cdot \text{sinc}^2\left(\frac{\ell x}{\lambda d}\right)$$



The major part of the energy is contained in the so-called the first or central lobe.

The angle ϑ_d that defines the central lobe is called "divergence angle":

$$\tan(\vartheta_d) = \frac{x_0}{d} = \frac{\lambda d}{d\ell} = \frac{\lambda}{\ell} \ll 1 \longrightarrow \text{paraxial condition}$$

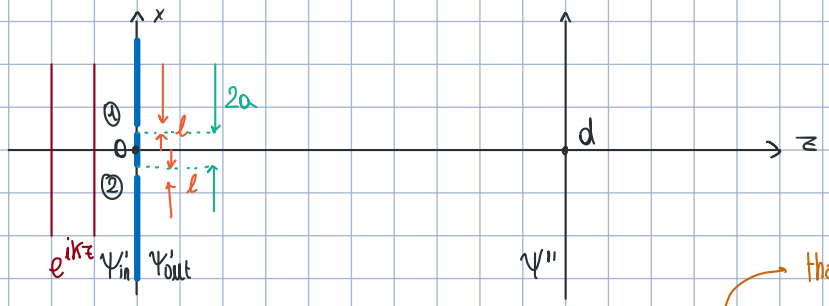
In paraxial condition, the divergence angle is small ($\vartheta_d \ll 1$ rad) and so we can approximate this angle with its tangent or sine:

$$\vartheta_d \simeq \tan\vartheta_d = \frac{\lambda}{\ell}$$

[e.g. $\lambda = 500$ nm, $\ell = 200$ μm $\longrightarrow$ $\vartheta \simeq \lambda/\ell = 2.5$ mrad $\ll 1$ rad]

$43.6 \cdot 10^{-6}$ °

2) DIFFRACTION OF LIGHT BY A PAIR OF SLITS:



thanks to linearity of the Maxwell's equations.

The result can be written with the principle of superposition: the total wave function is sum of the wave function of the first slit and the wave function of the second slit.

$$\Psi'' = \Psi''_{①} + \Psi''_{②}$$

$$\Psi'_{out_{①}} = \text{rect}\left(\frac{x-a}{\ell}\right)$$

$$\Psi''_{①} = \frac{\ell}{i\lambda d} e^{ikr_1} \text{sinc}\left[\frac{\ell}{\lambda d}(x-a)\right]$$

$$\Psi'_{out_{②}} = \text{rect}\left(\frac{x+a}{\ell}\right)$$

$$\Psi''_{②} = \frac{\ell}{i\lambda d} e^{ikr_2} \text{sinc}\left[\frac{\ell}{\lambda d}(x+a)\right]$$

$$\Rightarrow \Psi'' = \frac{\ell}{i\lambda d}\left[e^{ikr_1}\text{sinc}\left[\frac{\ell}{\lambda d}(x-a)\right] + e^{ikr_2}\text{sinc}\left[\frac{\ell}{\lambda d}(x+a)\right]\right] = \frac{\ell}{i\lambda d}\text{sinc}\left(\frac{\ell}{\lambda d}x\right)\left(e^{ikr_1} + e^{ikr_2}\right)$$

single-slit diffraction term

two wave interference term

In far field regime:

$$\frac{(\ell/2)^2}{\lambda d} \ll 1$$

we have $2a > \ell \longrightarrow a > \ell/2$. We have also consider that $\frac{a\ell}{\lambda d} \ll 1$

$$\longrightarrow a \ll \frac{\lambda d}{\ell} = x_0$$

The last lecture we've found the expression of the field after the two slits:

$$\Psi''(P) \cong \frac{\ell}{i\lambda d}\,\mathrm{sinc}\left[\frac{\ell}{\lambda d}x\right]\left(e^{ikr_1}+e^{ikr_2}\right)$$

The optical intensity is then:

$$I''(P) \propto |\Psi''(P)|^2$$

$$I''(P) \propto \mathrm{sinc}^2\left(\frac{\ell x}{\lambda d}\right)\cdot\left|e^{ikr_1}+e^{ikr_2}\right|^2$$

$$|a+b|^2 = (a+b)^*(a+b) = (a^*+b^*)(a+b) = a^*a + a^*b + ab^* + b^*b = |a|^2 + 2\,\mathrm{Re}\{a^*b\} + |b|^2$$

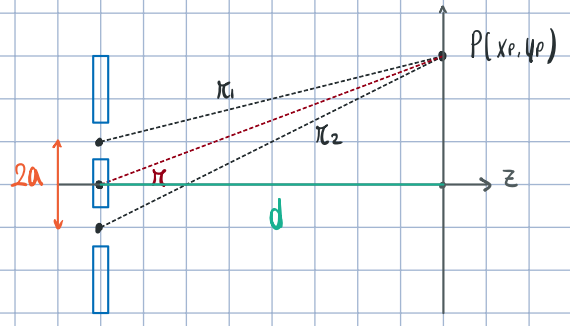
$$\left|e^{ikr_1}\right|^2 + 2\,\mathrm{Re}\left\{e^{-ikr_1}e^{ikr_2}\right\} + \left|e^{ikr_2}\right|^2 =$$

$$= 1 + 1 + 2\,\mathrm{Re}\left\{e^{ik(r_2-r_1)}\right\}$$

$$= 2 + 2\cos\left[k(r_2-r_1)\right] = 2\left\{1+\cos\left[k(r_2-r_1)\right]\right\}$$

$$\Rightarrow \quad I''(P) \propto \mathrm{sinc}^2\left(\frac{\ell x}{\lambda d}\right)\left\{1+\cos\left[k(r_2-r_1)\right]\right\}$$

will vary from 0 (destructive interference) to 2 (constructive interference).



$$r_1 = \sqrt{(x-a)^2+d^2} = d\sqrt{1+\left(\frac{x-a}{d}\right)^2}$$

small term (far-field approx.)

$$\simeq d\left[1+\frac{1}{2}\left(\frac{x-a}{d}\right)^2\right]$$

Taylor expansion truncated at the 2 term

$$r_2 = \sqrt{(x+a)^2+d^2} \simeq d\left[1+\frac{1}{2}\left(\frac{x+a}{d}\right)^2\right]$$

$$r_1 \cong d + \frac{(x-a)^2}{2d} = d + \frac{x^2-2ax+a^2}{2d}$$

$$r_2 \cong d + \frac{(x+a)^2}{2d} = d + \frac{x^2+2ax+a^2}{2d}$$

$$r_2 - r_1 \simeq \frac{4ax}{2d} = \frac{2ax}{d}$$

So the intensity is:

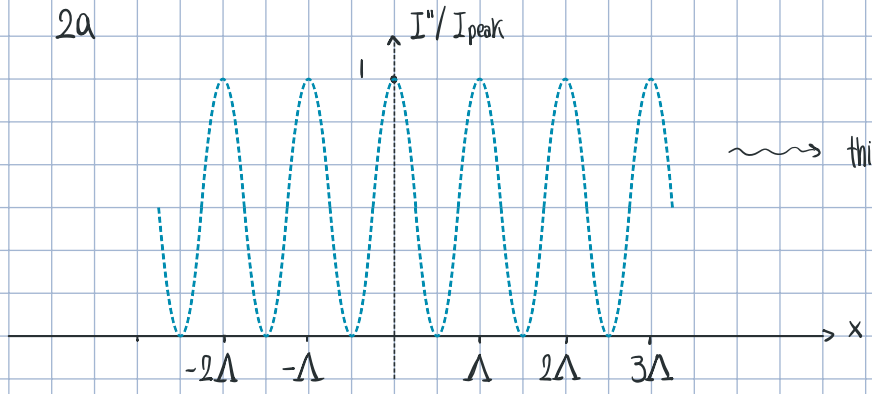
$$I''(P) \propto \mathrm{sinc}^2\left(\frac{\ell x}{\lambda d}\right)\left[1+\cos\left(2\pi\frac{2a}{\lambda d}x\right)\right]$$

$$I''(P) \cong I_{peak}\cdot\mathrm{sinc}^2\left(\frac{\ell x}{\lambda d}\right)\cdot\boxed{\frac{1}{2}\left[1+\cos\left(2\pi\frac{2a}{\lambda d}x\right)\right]}$$

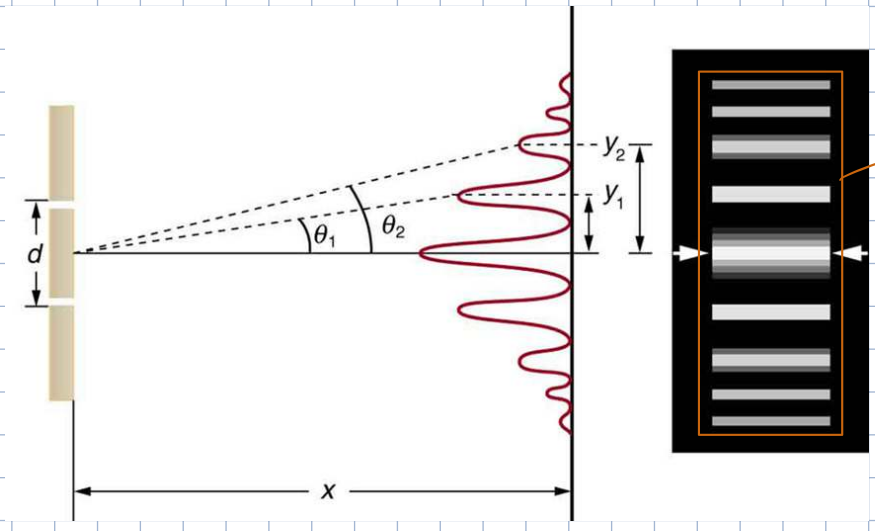
interference term from 0 to 1

The spatial period ("pitch") of the interference term is:

$$\Lambda = \frac{\lambda d}{2a}$$



↝ this has to be enveloped with the sinc^2

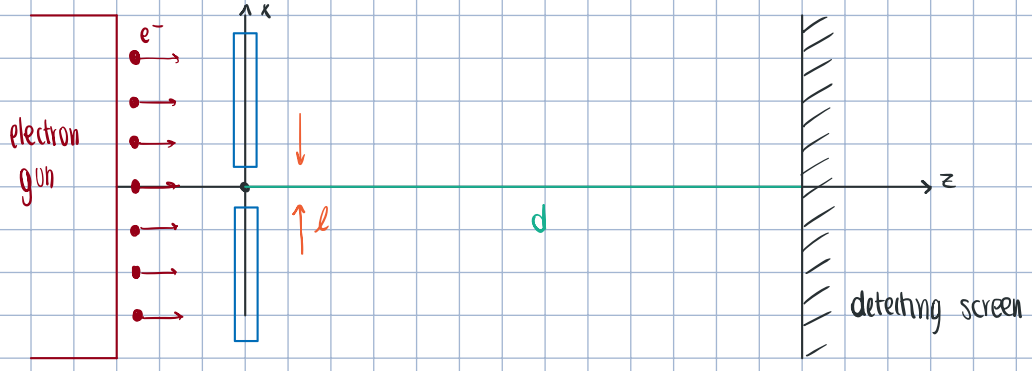


→ interference fringes.

This is the Young's experiment (1801) and it was a "proof" of wave theory light against corpuscolar theory of light (Newton, 18th century).

SINGLE SLIT EXERIMENT

It is a very similar experiment to the interference of light by a single slit, but this time we don't have a plane wave, but a stream of electrons that incide on the slit.



All the electrons with the same velocity (modulus is) along the x-axis.

We expect that only the electrons in line with the slit can arrive at the detecting screen → we expect a rectangular distribution with a width equal to the width of the slit.

Instead, experimentally, we find a cardinal sine distribution similar to the diffraction of the plane wave, with a λ, called De-Broglie wavelenght, as follow:

$$\lambda = \frac{h}{p} = \frac{h}{m v}$$ where $h \triangleq$ Planck's constant $\cong 6.63 \cdot 10^{-34}$ J·s

↳ indicates an action = position · momentum = energy · time

IF the Plank's constant would be 0, the experiment would give us the intuitive result of no-interference.

e.g. $\lambda = 0.5\ \mu m$, $v = ?$ $\Rightarrow$ $\lambda = \frac{h}{m v}$ → $v = \frac{h}{m \lambda} = 1.455 \cdot 10^{3}$ m/s

Probability density function of detecting an electron at the position x on the detecting screen:

$$P(x) \propto \operatorname{sinc}^2\left(\frac{\ell}{\lambda d} x\right) \quad \text{with} \quad \lambda = \frac{h}{m_e v}$$

We have no electrons for $x = \pm x_0, \pm 2x_0, \pm 3x_0, \dots$

This is a manifestation of the dualism wave-particle of quantum physics.

COMPLEMENTARY PRINCIPLE (Bohr - 1928)

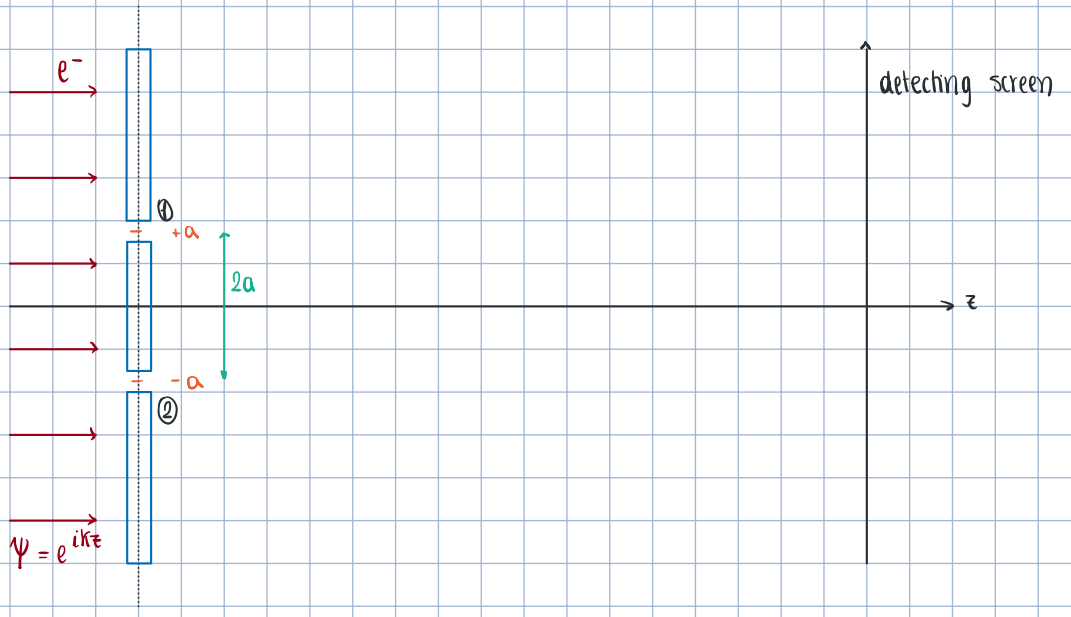
- wave-particle duality
- "complementary" of conjugate physical quantities

The electron diffraction and interference is described by the "Double slit experiment".

The situation is equivalent to the Young's experiment with plane waves, and works even with one electron at the time. This experiment is also known as the "which-way" experiment. This because we can not know in which slit the electron will pass through.

So the electron is described by a wave function $\Psi(x,y,z)$ and the probability density function of measuring (detecting) the electron in a point $P(x,y,z)$ is $|\Psi(x,y,z)|^2$.

ELECTRON DOUBLE SLIT EXPERIMENT ⟶ "WHICH-WAY EXPERIMENT"



$$\lambda = \frac{h}{p} = \frac{h}{m_e v} \longrightarrow p = \frac{h}{\lambda} = \frac{h}{2\pi/k} = \frac{h}{2\pi} k = \hbar k$$

↳ reduced Plank's constant ("h-bar")

We can consider at first the situation where the second slit is closed: on the detecting screen we have the diffraction figure of the slit 1. The probability to find the electron on the detecting screen is given by:

$$P_1(x) = C \cdot \operatorname{sinc}^2\left[\frac{\ell}{\lambda d}(x-a)\right]$$

normalization constant ⟶ $\int_{-\infty}^{+\infty} P_1(x)\,dx = 1 \Rightarrow C = \dots$

We can then consider the other case: slit 1 closed while the slit 2 is open.

$$P_2(x) = C \cdot \operatorname{sinc}^2\left[\frac{\ell}{\lambda d}(x+a)\right]$$

If both the slits are open at the same time there is interference and the total probability is not simply the sum of the two single probabilities:

$$P(x) \neq P_1(x) + P_2(x)$$

$$P(x) = |\psi''(x)|^2 = |\psi_1''(x) + \psi_2''(x)|^2$$

SUPERPOSITION PRINCIPLE OF QUANTUM STATES: $\psi''(x) = \psi_1''(x) + \psi_2''(x)$

In general, $|\psi''(x)|^2 = |\psi_1''(x) + \psi_2''(x)|^2 \neq |\psi_1''(x)|^2 + |\psi_2''(x)|^2$ due to quantum interference!

The total probability can be approximated by the following expression, when $x_0 \gg \Lambda$ ($\ell \ll 2a$):

$$P(x) \simeq C \cdot \mathrm{sinc}^2\left(\frac{\ell x}{\lambda d}\right) \cdot \frac{1}{2}\left[1 + \cos\left(2\pi \frac{2a}{\lambda d} x\right)\right]$$

$\Lambda = \frac{\lambda d}{2a}$

In case of no-path information, the electron is in a superposition of two quantum states:

1) electron passing through slit 1;

2) electron passing through slit 2.

On the detecting screen, the electron will be detected in a unique position (like classical particle), but with a probability distribution showing interference fringes (like a classical wave) due to quantum interference.

It is possible to destroy the quantum interference by inserting two detector (path detector) in each slit.

↓ will detect only the passage of the electron, without absorb or destroy it

In this case we observe that the electron can either pass through the slit nr. 1 or the slit nr. two, and so we cannot see the passage through both slits. Moreover the interference is destroyed and the zero probability points on the detecting screen are no-more visible

quantum state reduced to state 1 — quantum state reduced to state 2

there is no more superposition

If the path-detectors are not so efficcent the interferenie fringes are still visible, even if the zero-points are nomore "zero", but a value slightly larger.

In the case of two path-detectors in the slits we have

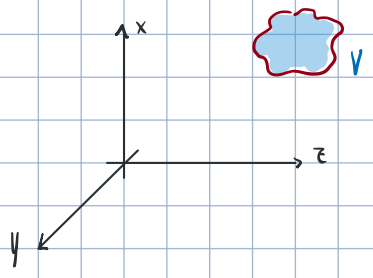
$$P(x) = \frac{1}{2}\left[P_1(x) + P_2(x)\right] \simeq \frac{1}{2}\,\mathrm{sinc}^2\left[\frac{\ell x}{\lambda d}\right]$$

⇒ Principle of COMPLEMENTARITY (Bohr - 1927) ⟶ Wave-Particle Duality.

The path-detector can be implemented by using a Wilson chamber (~1899). This chamber is usable with all charged particles, like electrons for our case. The chamber is transparent and filled with saturated vapor. When a charged particle pass through this vapor, it creates, due to its charge, an ion that quickly becomes a condensation point for the vapor. What we see is a trace in the vapor, that indicates the path used by the electron.

It's important also to talk about the "Copenhagen interpretation" of quantum physics: it's a statistical interpretation using the concept of the wave function $\Psi(x,y,z)$. The quantum state of a particle (eg. electron, protons, atoms, ions, particles) is described by the wave function $\Psi(x,y,z)$ and the probability density function of detecting the particle in a point $P(x,y,z)$ is given by

$$P(x,y,z) = |\Psi(x,y,z)|^2$$



The probability of finding the particle in a volume V is

$$\iiint_V |\Psi(x,y,z)|^2 \, dx\, dy\, dz$$

We have also find that for an electron (particle) with a well-defined value of momentum:

$$\vec{p} = m_e \cdot \vec{v}$$ aligned with z-axis

$$|\vec{p}| = p = m_e v$$

the wave function describing this state is given by a plane wave

$$\Psi(z) = C \cdot e^{ikz}$$

with the De-Broglie wavelenght relation $p = \hbar k$:

$$\Psi(z) = C \cdot e^{\frac{ipz}{\hbar}}$$

$$|\Psi(z)|^2 = |C|^2 \longrightarrow$$ not dependent on x,y,z!

↳ in this case the wave function is not normalizable

There is a complete delocalization, so there is the same probability to find the electron everywhere.

The mechanical quantities which are canonically conjugate are complementary in quantum physics:

x, p_x
y, p_y
z, p_z
t, E

} are pairs of complementary quantities.

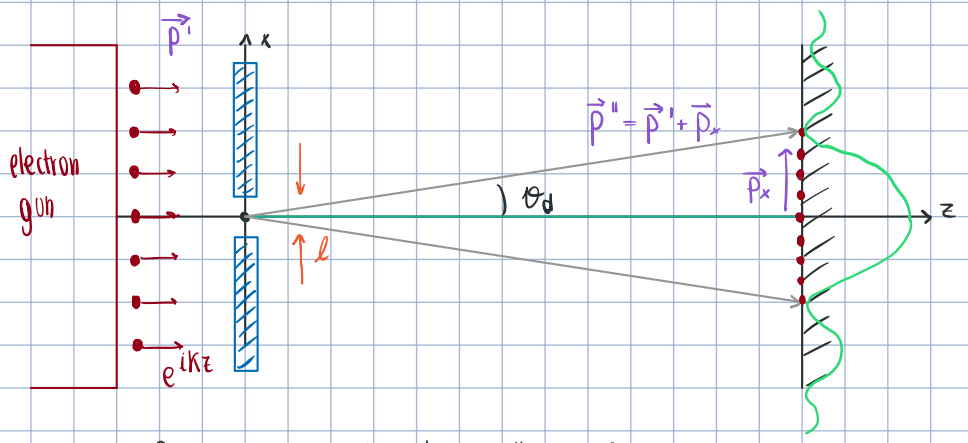
Complementarity means that it's not possible to simultaneously have well-defined values for a pair of complementary physical values.

UNCERTAINTY PRINCIPLE (Heisenberg, 1927)

For complementary physical quantities:

$$\Delta x \cdot \Delta p_x \geq \frac{\hbar}{2}$$

It's another manifestation of the complementary principle.



The action of the slit is to bring the perfectly delocalized wave function into a central lobe, with the drawback of having an additional momentum component to the final momentum vector.

$$\psi' = C \cdot \text{rect}\left(\frac{x}{\ell}\right)$$

$$\psi' \neq 0 \quad \text{for} \quad -\ell/2 < x < \ell/2 \longrightarrow -\Delta x < x < +\Delta x \Rightarrow \Delta x \simeq \ell/2$$

The slit introduces an incertainty on the position, and so on the momentum:

$$\Delta p_x \simeq p \cdot \tan\vartheta_d \simeq p \cdot \vartheta_d = p\frac{\lambda}{\ell} \longrightarrow \Delta p_x \simeq p\frac{\lambda}{2\cdot\Delta x}$$

$\ell \simeq 2\Delta x$

$$\Rightarrow \Delta x \cdot \Delta p_x \simeq \frac{\lambda p}{2} = \frac{h}{2} > \frac{\hbar}{2}$$

$\lambda = \frac{h}{p}$

UNCERTAINTY HEISENBERG PRINCIPLE IMPLICATIONS

We may want to apply the uncertainty principle to a macroscopic body, such as a tennis ball:

- uncertainty in position $\Delta x = 1\ \mu m$.

We want to calculate the uncertainty in the velocity from the momentum:

$$\Delta x \cdot \Delta p_x \approx \frac{h}{2} \longrightarrow \Delta p_x \sim \frac{h/2}{\Delta x} = \frac{6.63 \cdot 10^{-34}\ Js}{2\,(1 \cdot 10^{-6}\ m)} \simeq 3 \cdot 10^{-28}\ Kg \cdot m \cdot s^{-1}$$

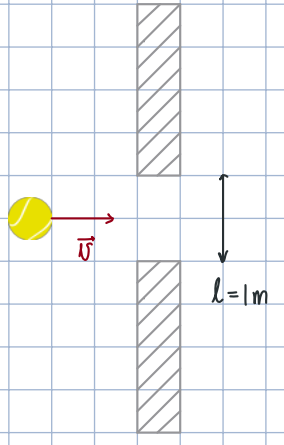
$$p_x = m v_x \longrightarrow \Delta v_x = \frac{\Delta p_x}{m} = \frac{3 \cdot 10^{-28}\ Kg \cdot m \cdot s^{-1}}{6 \cdot 10^{-2}\ Kg} = \boxed{5 \cdot 10^{-27}\ m s^{-1}}$$ Negligible!

↳ in case of electrons the mass is really small ⇒ the uncertainty on the velocity is no more negligible

The implications of the Heisenberg principle for the macroscopic (classical physics) are irrelevant!

It is possible to say that classical mechanics can be obtained from quantum mechanics in the limit of $h \longrightarrow 0$. The classical mechanics is a "very good" approximation of quantum mechanics when the product between typical tollerances in measuring a pair of canonically conjugated physical quantities (e.g. Position-Momentum) must be much higher than the Plank's constant.

E.g.: tennis ball passing through a slit



$v = 108\ Km \cdot h^{-1} = 30\ m s^{-1}$ $\quad m = 60g = 6 \cdot 10^{-2}\ Kg$

$\lambda \triangleq$ de-Broglie wavelength $= \frac{h}{p} = \frac{h}{mv} \simeq 3 \cdot 10^{-34}\ m$

$\vartheta_d \triangleq$ diffraction angle $\simeq \frac{\lambda}{\ell} \cong 3 \cdot 10^{-34}$ rad

SCHRÖDINGER WAVE EQUATION

Waves of matter (or also "matter wave") are described by wave functions $\Psi(x,y,z)$.

We know by classical optics that monochromatic waves in "free propagation" are described by a scalar envelope $\Psi(x,y,z)$, obeying the Helmholtz equation:

$$\nabla^2 \Psi(x,y,z) + K^2 \Psi(x,y,z) = 0$$

where $K \triangleq$ modulus of the wave vector $= \frac{2\pi}{\lambda} = \frac{2\pi}{\lambda_0} n$ (uniform medium so it's constant in all the points.)

with suitable boundary conditions

The Laplacian operator: $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

$$\nabla^2 \Psi(x,y,z) = \frac{\partial^2}{\partial x^2}\Psi(x,y,z) + \frac{\partial^2}{\partial y^2}\Psi(x,y,z) + \frac{\partial^2}{\partial z^2}\Psi(x,y,z)$$

plane wave solution: $\Psi = C \cdot e^{iKz}$

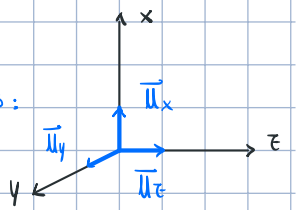
We can easily verify that the plane wave is a solution of Helmholtz equation:

$$\nabla^2 \left(C e^{iKz} \right) = C \frac{\partial^2}{\partial z^2} e^{iKz} = C \frac{\partial}{\partial z}\left(\frac{\partial}{\partial z} e^{iKz} \right) = C \cdot iK \frac{\partial}{\partial z}\left(e^{iKz}\right) = C \cdot (iK)^2 \cdot e^{iKz}$$

$$= -CK^2 e^{iKz}$$

$$\Rightarrow \left(-CK^2 e^{iKz}\right) + K^2 \left(C e^{iKz}\right) = 0 \quad \checkmark \text{ Verified!}$$

Versors:



This is also satisfied for a generic wave-vector ($\longrightarrow$ any direction): $\vec{K} = K_x \vec{u}_x + K_y \vec{u}_y + K_z \vec{u}_z$.

In case of a generic plane wave vector:

$$\Psi(x,y,z) = C \cdot e^{iK_x x} \cdot e^{iK_y y} \cdot e^{iK_z z} = C e^{i(K_x x + K_y y + K_z z)} = C e^{i\vec{K}\cdot\vec{x}}$$

$\vec{x}$ → position vector: $\vec{r}_p = (x_p, y_p, z_p)$, $P(x_p, y_p, z_p)$

$$K^2 = |\vec{K}|^2 = K_x^2 + K_y^2 + K_z^2$$

The solutions of the Helmholtz equation are eigenfunction of the laplacian operator ∇^2, with eigenvalues $-K^2$.

> If I consider an operator $\hat{M}$, I can write an eigenvalue equation:
>
> $\hat{M}\Psi = m\Psi$
>
> If the equality is satisfied we can say that Ψ is EIGENFUNCTION of $\hat{M}$ and m is EIGENVALUE of $\hat{M}$.

$\nabla^2 \Psi(x,y,z) = -K^2 \Psi(x,y,z)$ $\rightsquigarrow$ Helmholtz eq. written as eigenvalue equation

$\Rightarrow$ the envelope $\Psi(x,y,z)$ are eigensolutions and eigenfunctions of ∇^2, with corresponding eigenvalues K^2.

Only for the plane waves, is also eigenfunction of the differential vectorial operator: the GRADIENT

$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$ where ∇ is the "nabla" operator

$$\nabla \Psi(x,y,z) = \text{grad}(\Psi) = \frac{\partial \Psi}{\partial x}\vec{u}_x + \frac{\partial \Psi}{\partial y}\vec{u}_y + \frac{\partial \Psi}{\partial z}\vec{u}_z$$

E.g.: plane wave

$$\Psi = e^{i\vec{K}\cdot\vec{r}} = e^{iK_x x} e^{iK_y y} e^{iK_z z}$$

$$\frac{\partial}{\partial x}\Psi(x,y,z) = iK_x e^{iK_x x} e^{iK_y y} e^{iK_z z} = iK_x \cdot \Psi$$

$\vdots$

Only the plane wave is eigenfunction of $\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}$ with eigenvalue iK_x, iK_y, iK_z.

$$\nabla\Psi(x,y,z) = \left(\frac{\partial \Psi}{\partial x}, \frac{\partial \Psi}{\partial y}, \frac{\partial \Psi}{\partial z}\right) = \left(iK_x\Psi, iK_y\Psi, iK_z\Psi\right) = \left(iK_x, iK_y, iK_z\right)\Psi = i\vec{K}\Psi$$

The gradient of the wave function Ψ is equal by the product of i, the wave vector and Ψ $\Rightarrow$ the plane-wave function Ψ is eigenfunction of ∇ with (vectorial) eigenvalue $i\vec{K}$

In quantum physics, the quantum state of a matter wave (e.g. an electron) with a well-defined value $\vec{p}$ of momentum is described by a "plane-wave like" wave function

$\Psi(x,y,z) = e^{i\vec{K}\cdot\vec{r}}$ where $\boxed{\vec{p} = \hbar\vec{K}}$ de-Broglie relation $\longrightarrow \lambda = \frac{h}{p}$

$\downarrow$

$= e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$

But the gradient of Ψ is:

$$\nabla\Psi = i\vec{K}\Psi = \frac{i}{\hbar}\vec{p}\Psi \longrightarrow \boxed{-i\hbar\nabla\Psi = \vec{p}\Psi}$$ Eigenvalue equation

The well-defined value $\vec{p}$ of the momentum for the particle is eigenvalue of $-i\hbar\nabla$.

In quantum physics, the momentum is described by the operator:

$$-i\hbar\nabla = \left(-i\hbar\frac{\partial}{\partial x}, -i\hbar\frac{\partial}{\partial y}, -i\hbar\frac{\partial}{\partial z}\right)$$

CLASSICAL MECHANICS (dynamical quantities)	QUANTUM PHYSICS (operators)
p_x	$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$
p_y	$\hat{p}_y = -i\hbar \frac{\partial}{\partial y}$
p_z	$\hat{p}_z = -i\hbar \frac{\partial}{\partial z}$
$\vec{p} = (p_x, p_y, p_z)$	$\hat{\vec{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z) = -i\hbar\nabla$

The last time we have seen that the momentum in quantum mechanics can be represented by the operator

$$\hat{\vec{p}} = -i\hbar\nabla$$

in the position - representation where the quantum state is described by the wave function $\Psi(x,y,z)$.

$$\hat{\vec{p}}\,\Psi(x,y,z) = -i\hbar\nabla\Psi(x,y,z).$$

We now consider the so-called "Free particle" (that is a particle in a region without external forces). In classical physics the energy of this particle is constant (= no change during evolution) and it is given by the expression

$$E = E_{kin} = \frac{1}{2}mv^2$$

$$p = mv \longrightarrow \boxed{E = \frac{1}{2}\cdot\frac{p^2}{m}}$$

In quantum physics we can substitute the momentum p with its operator and obtain the energy operator, the so-called "Hamiltonian operator" or "Energy operator":

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

$$\hat{p}^2 = (-i\hbar)^2\cdot\nabla^2 = -\hbar^2\nabla^2$$

(∇^2 → Laplacian)

$$\hat{\vec{p}} = \left(-i\hbar\frac{\partial}{\partial x}, -i\hbar\frac{\partial}{\partial y}, -i\hbar\frac{\partial}{\partial z}\right) = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$$

In classical physics:

$$p^2 = |\vec{p}|^2 = p_x^2 + p_y^2 + p_z^2$$

If we move this relation in quantum mechanics:

$$\hat{p}^2 = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2 = (-i\hbar)^2\underbrace{\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]}_{\text{LAPLACIAN OPERATOR: } \nabla^2} = (-i\hbar)^2\nabla^2 = -\hbar^2\nabla^2$$

$$\hat{p}^2\Psi(x,y,z) = -\hbar^2\nabla^2\Psi(x,y,z)$$

The Hamiltonian operator for the "free" particle is:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2$$

For a free particle the quantum state with well-defined momentum vector $\vec{p}$ is described by a "plane-wave like" wave function:

$$\Psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} = e^{i\frac{\vec{p}}{\hbar}\cdot\vec{r}}$$

In this case, if the momentum of the particle is precise, also the energy is well-defined. The wave function is eigenfunction of the momentum operator $\vec{p}$ and also eigenfunction of the Hamiltonian operator $\hat{H}$ (because well-defined $\vec{p}$ $\Rightarrow$ well-defined energy E).

The eigenvalue of this $\Psi(\vec{r})$ for $\hat{H}$ is exactly

$$E = \frac{1}{2}\cdot\frac{p^2}{m} = \frac{1}{2}\cdot\frac{|\vec{p}|^2}{m}$$

$$\hat{H}\Psi = E\Psi \longrightarrow \text{Schrödinger equation}$$

For a free-particle the stationary (with probability density function $|\Psi|^2$ time-indipendent) states are described by wave functions $\Psi(x,y,z)$ solving the TIME-INDIPENDENT SCHRÖDINGER EQUATION.

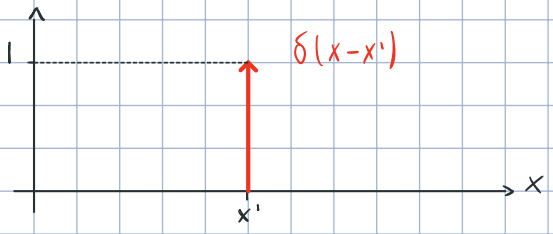
The stationary states of any quantum systems are eigensolutions of the hamiltonian operator with eigenvalues given by the energy.

The states with a well-defined position (the so-called "well localized position") $\vec{r}' = (x',y',z')$ will be described by a wave-function given by a Dirac's delta centered in (x',y',z'):

$$\Psi(x,y,z) = \delta(x-x', y-y', z-z')$$

$$= \delta(x-x')\cdot\delta(y-y')\cdot\delta(z-z') = \begin{cases} \infty & \text{for } x=x', y=y', z=z' \\ 0 & \text{otherwise} \end{cases}$$

The monodimensional case can be represented as follows:



Property: $f(x)\cdot\delta(x-x') = f(x')\cdot\delta(x-x')$

The quantum operator $\hat{x}$ can be identified with the product $x\cdot$:

$$\hat{x}\,\Psi(x,y,z) = x\cdot\Psi(x,y,z)$$

In this case the well-localized state with position x' is an eigenfunction of $\hat{x}$ with eigenvalue x'.

$$\hat{x}\,\delta(x-x') = x\cdot\delta(x-x') = x'\cdot\delta(x-x')$$

In the 3-dimensional case:

$$\hat{x}\cdot\delta(x-x',y-y',z-z') = x'\cdot\delta(x-x',y-y',z-z')$$

$$\hat{y}\cdot\delta(x-x',y-y',z-z') = y'\cdot\delta(x-x',y-y',z-z')$$

$$\hat{z}\cdot\delta(x-x',y-y',z-z') = z'\cdot\delta(x-x',y-y',z-z')$$

The position operator

$$\hat{\vec{r}} = (\hat{x},\hat{y},\hat{z}) \quad\Longleftrightarrow\quad \vec{r}\cdot = (x,y,z)$$

$$\hat{\vec{r}}\,\Psi(\vec{r}) = \vec{r}\,\Psi(\vec{r}) = (x\Psi, y\Psi, z\Psi)$$

Any physical quantity of classical mechanics can be written as

$$M(\vec{r},\vec{p},t)$$

If we move to quantum mechanics, the observable is described by the operator

$$\hat{M} = M(\hat{\vec{r}},\hat{\vec{p}},t) \qquad \text{with } \hat{\vec{r}} = \vec{r}\cdot \text{ and } \hat{\vec{p}} = -i\hbar\nabla$$

The energy of free particle

- classical physics: $E = \dfrac{p^2}{2m}$
- quantum physics: $\hat{H} = \dfrac{\hat{p}^2}{2m}$

In the general case of a particle in a conservative field of forces we have that

$$E_{tot} = E_{kin} + E_{pot} = \frac{p^2}{2m} + V(\vec{r},t)$$

In quantum mechanics we have the hamiltonian operator:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r}, t) = -\frac{1}{2}\frac{\hbar^2}{m}\nabla^2 + V(\vec{r}, t)$$

We can now write the TIME-INDEPENDENT SCHRÖDINGER'S EQUATION

$$\hat{H}\Psi(\vec{r}) = E\Psi(\vec{r})$$

$$\downarrow$$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r}) + V(\vec{r}, \cancel{t})\cdot\Psi(\vec{r}) = E\Psi(\vec{r})$$

time-independent

Differential equation (solved imposing the boundary conditions)

We want now to analyze the MEASUREMENT PROCESS.

In classical physics the measurement process is NEUTRAL (i.e. the measurement does not perturb in principle the measured properties of the object), so the measurement results are (in principle) indipendent by the measurement device/process. Indeed, there is a small error in the measurement due to the limited precision of the measurement device (but there is no theoretical limit; increasing precision, the error tends to zero). We can measure at a given instant of time, position $\vec{r}$ and momentum $\vec{p}$ (velocity) of any macroscopic body, and then in a deterministic way we can calculate the motion of the body and its trajectory.

On the other hand, in quantum physics the measurement process is NOT NEUTRAL ("not neutral observer") that is strictly perturbs the system. In quantum physics, the physical properties of the system are influenced (in a theoretical way) by the observer → any measurement device producing a macroscopic result

The quantum measurement process is random and irreversible (not reversible):

- RANDOM: the knowledge of the quantum states (e.g. described by $\Psi(x,y,z)$) defines the probabilities of occurrence of the possible results of a measurement.
- IRREVERSIBLE: there is not an inverse process recovering the initial state from the state obtained after the measurement. There is not (in general) an inverse operator cancelling the measurement process: $\Psi_{out} \not\rightarrow \Psi_{in}$ (apart some particular cases).

TIME-DEPENDENT SCHRÖDINGER'S EQUATION (1926)

$$\hat{H}\,\Psi(\vec{r},t) = i\hbar\,\frac{\partial}{\partial t}\,\Psi(\vec{r},t)$$

We have seen that a free-particle with a well-defined momentum $p = \hbar k$, and hence also well-defined energy $E = E_{kin} = \frac{p^2}{2m}$, is described by a stationary quantum state with wave function

$\Psi(z) = c\cdot e^{ikz}$ (plane wave, e.g. propagating along the z-axis).

We can consider a "monochromatic" plane-wave with Plank's relation (1901):

$$E = h\nu = \hbar\omega$$

[Firstly introduced by Plank for explaining the issue of the radiation of the black body].

In the following years, this energy has been recognised also as the single photon energy.

The monochromatic plane wave for free particle of energy E:

$$\Psi(z,t) = c\cdot e^{i(kz-\omega t)} = c\cdot e^{ikz}\,e^{-i\omega t} = \Psi(z)\cdot e^{-i\omega t}$$

↓ using Plank's equation

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

$$\frac{\partial}{\partial t}\Psi(z,t) = \Psi(z)\,\frac{\partial}{\partial t}\,e^{-i\frac{E}{\hbar}t} = \Psi(z)\left(-i\frac{E}{\hbar}\right)e^{-i\frac{E}{\hbar}t} = -i\frac{E}{\hbar}\,\Psi(z,t) = -i\omega\,\Psi(z,t) \quad (1)$$

$$\hat{H}\,\Psi(z,t) = \hat{H}\,\Psi(z)\cdot e^{-i\frac{E}{\hbar}t}$$

We assume now $\hat{H}$ time-independent:

$$\hat{H}\,\Psi(z,t) = e^{-i\frac{E}{\hbar}t}\cdot\hat{H}\,\Psi(z)$$

$$\Psi(z) = c\cdot e^{ikz} = e^{i\frac{p}{\hbar}z}$$

is an eigenfunction of $\hat{p}^2$ ⟶ for a free particle $E = \frac{p^2}{2m}$.

$$\hat{H} = \frac{\hat{p}^2}{2m}$$ (no potential energy in this case!)

$\Psi(z) = c\cdot e^{ikz}$ is also eigenfunction of $\hat{H}$:

$$\hat{H}\,\Psi(z) = E\,\Psi(z)$$

that is $\Psi(x)$ is a solution of the time-independent Schrödinger equation.

We have:

$$\hat{H}\Psi(x,t) = e^{-i\frac{E}{\hbar}t}\, E\,\Psi(x) = E\,\Psi(x,t) \qquad (2)$$

We can compare the expression (1) and (2):

$$\begin{cases} (1)\ \dfrac{\partial}{\partial t}\Psi(x,t) = -i\dfrac{E}{\hbar}\Psi(x,t) \\ (2)\ \hat{H}\Psi(x,t) = E\,\Psi(x,t) \end{cases}$$

are equal

$$\Rightarrow \quad \frac{\partial}{\partial t}\Psi(x,t) = -\frac{i}{\hbar}\hat{H}\Psi(x,t) \longrightarrow \boxed{\hat{H}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)}$$

Time-dependent Schrödinger's equation

It is possible to extend this equation at all kind of wave function, and not only at monochromatic wave function.

In general, for any particle of non-relativistic (has to be applied only when the velocity is $\ll c$) quantum mechanics we have that in the position-representation the knowledge of the wave function $\Psi(\vec{x},t)$ for $t = t_0$ and of the Hamiltonian of the system:

$$\hat{H}(\hat{\vec{x}},\hat{\vec{p}},t) = \frac{\hat{p}^2}{2m} + V(\hat{\vec{x}},t) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x},t)$$

For any time $t \geq t_0$, then it is possible to determine $\Psi(\vec{x},t)$ just solving the Schrödinger equation:

$$\hat{H}\Psi(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{x},t)$$

We assume now a potential energy $V(\vec{x})$ time-independent (i.e. time-independent conservative field of forces, considered according to classical physics):

$$\vec{F}(\vec{x}) = -\nabla V(\vec{x})$$

both are from "classical physics"

$$\Downarrow$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{x}) \qquad \text{(time independent)}$$

$$\frac{\partial}{\partial t}\Psi(\vec{r},t) = -\frac{i}{\hbar}\hat{H}\Psi(\vec{r},t)$$

This is a very simple first order linear differential equation with constant coefficients:

$$\begin{cases} \frac{d}{dt}f(t) = a\cdot f(t) \\ f(t)\big|_{t=t_0} = f(t_0) \end{cases} \xrightarrow{\text{solution}} f(t) = f(t_0)\, e^{a(t-t_0)}$$

By similarity we can write the solution of the Schrödinger equation:

$$\Psi(\vec{r},t) = \underbrace{e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}}_{\text{TIME-EVOLUTION OPERATOR}}\Psi(\vec{r},t_0)$$

The eigenfunction of the Hamiltonian are characterized by a well-defined energy E (eigenvalue):

$$\hat{H}\Psi_E(\vec{r}) = E\Psi_E(\vec{r})$$

↳ "well-defined" energy

We assume now:

$$\Psi(\vec{r},t_0) = \Psi_E(\vec{r})$$

$$\Psi(\vec{r},t) = e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}\cdot\Psi(\vec{r})$$

If Ψ is eigenfunction of an operator $\hat{A}$ (with eigenvalue a) then Ψ is also eigenfunction of $g(\hat{A})$, with eigenvalue $g(a)$.

$\Psi_E(\vec{r})$ is eigenfunction of $e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}$, with eigenvalue $e^{-\frac{i}{\hbar}(t-t_0)\cdot E}$

$$\Rightarrow \quad \Psi(\vec{r},t) = \Psi_E(\vec{r})\cdot e^{-\frac{i}{\hbar}E(t-t_0)}$$

e.g. $t_0 = 0$, or equivalently multiplying Ψ by $e^{-\frac{i}{\hbar}Et_0}$

(the quantum state is described by wave function apart for a multiplicative complex coefficient)

$\Psi(\vec{r},t)$ and $c\cdot\Psi(\vec{r},t)$ describe the same quantum state!

$$\boxed{\Psi(\vec{r},t) = \Psi_E(\vec{r})\cdot e^{-\frac{i}{\hbar}Et}}$$

Stationary state (the quantum state does not change during time)

E.g.: $|\Psi(\vec{r},t)|^2 = \left|\Psi_E(\vec{r})\cdot e^{-\frac{i}{\hbar}Et}\right|^2 = |\Psi_E(\vec{r})|^2 \longrightarrow$ time-independent!

SPECTRUM OF AN OPERATOR

The spectrum of an operator is defined as the set of its eigenvalues.

SPECTRUM OF AN OBSERVABLE:

(for example the Hermitian operator) is real-valued (collection of the possible results of measurement of the observable).

The spectrum of the hermitian operator can be of two kinds:

- discrete: finite or countable infinite number of eigenvalues;
- continuous: non-countable infinite number of eigenvalues.
- mixed discrete / continuous.

In case of the hamiltonian operator for a quantum-mechanical system, the spectrum (for energy eigenvalues) is discrete for bounded states (harmonic oscillator, an electron in atom, an electron in a molecule) while is continuous for unbounded states (e.g. free particle).

It is possible to build a complete orthogonal basis for the Hilber space describing a quantum system considering the eigenfunction of the Hamiltonian.

We can expand a generic wave function as superposition of eigenfunctions of $\hat{H}$ (that is stationary states with a well-defined energy).

(Discrete spectrum of $\hat{H}$):

$$\hat{H}\Psi_n(\vec{r}) = E_n\Psi_n(\vec{r}) \qquad (n = 0, 1, 2, 3, \dots \text{ non-negative integer})$$

$$\Psi(\vec{r},0) \equiv \Psi(\vec{r}) = \sum_n a_n \Psi_n(\vec{r})$$

a_n: scalar (complex) coefficient

(Continuous spectrum):

$$\Psi(\vec{r},0) \equiv \Psi(\vec{r}) = \int a_\alpha \Psi_\alpha(\vec{r})\, d\alpha$$

$$\hat{H}\Psi_\alpha(\vec{r}) = E_\alpha \Psi_\alpha(\vec{r}) \qquad (\alpha \text{ is a real number varying in a continuous interval})$$

In the discrete spectrum we can write the Schrödinger equation

$$\Psi(\vec{r},t) = \underbrace{e^{-\frac{i}{\hbar}t\hat{H}}}_{\text{linear operator}} \cdot \sum_n a_n \psi_n(\vec{r}) = \sum_n a_n e^{-\frac{i}{\hbar}t\hat{H}} \psi_n(\vec{r}) = \sum_n a_n e^{-\frac{i}{\hbar}tE_n} \psi_n(\vec{r})$$

$\Psi(\vec{r},t)$ is in general TIME-DEPENDENT, so $|\Psi(\vec{r},t)|^2$ is time dependent.

The quantum state is time independent only when the initial wave function is an eigenfunction of $\hat{H}$

$$\Psi(\vec{r},t) = \psi_n(\vec{r}) \cdot e^{-\frac{i}{\hbar}E_n \cdot t}$$

This is a stationary state.

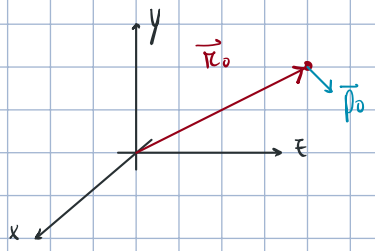
$$\hat{H}\Psi(\vec{r},t) = \hat{H}\psi_n(\vec{r}) \cdot e^{-\frac{i}{\hbar}tE_n} = e^{-\frac{i}{\hbar}E_n \cdot t} \hat{H}\psi_n(\vec{r}) = e^{-\frac{i}{\hbar}E_n t} E_n \psi_n(\vec{r}) = E_n \Psi(\vec{r},t)$$

CLASSICAL CASE

Single body of mass m. We know position and momentum at the initial time t_0:

$$\vec{r}(t_0) = \vec{r}_0$$

$$\vec{p}(t_0) = \vec{p}_0$$



The position and the momentum at any time can be evaluated through the Newton's second law:

$$\vec{F}(\vec{r},t) = m\vec{a}(t)$$

$$\boxed{\vec{F}(\vec{r},t) = m \cdot \frac{d^2}{dt^2}\vec{r}(t)} \longrightarrow \text{second-order differential equation}$$

With initial conditions:

$$\begin{cases} \vec{r}(t_0) = \vec{r}_0 \\ \vec{v}(t_0) = \dfrac{d}{dt}\vec{r}(t)\Big|_{t=t_0} = \dfrac{\vec{p}_0}{m} \end{cases}$$

QUANTUM MECHANICS

For a single quantum particle of mass m (for instance electron, atom, etc....) at initial time t_0 we know the quantum state expressed by the wave function $\Psi(x,y,z)$. So we know the probability distribution of the particle in the space.

$|\Psi(x,y,z)|^2$ is the probability density function of finding the particle at point $P(x,y,z)$

$$\Downarrow$$

It is possible to determine the evolution of the wave function for $t \geq t_0$ in a deterministic way (but in absence of measurements !), solving the Schrödinger's equation:

$$\hat{H}\Psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)$$

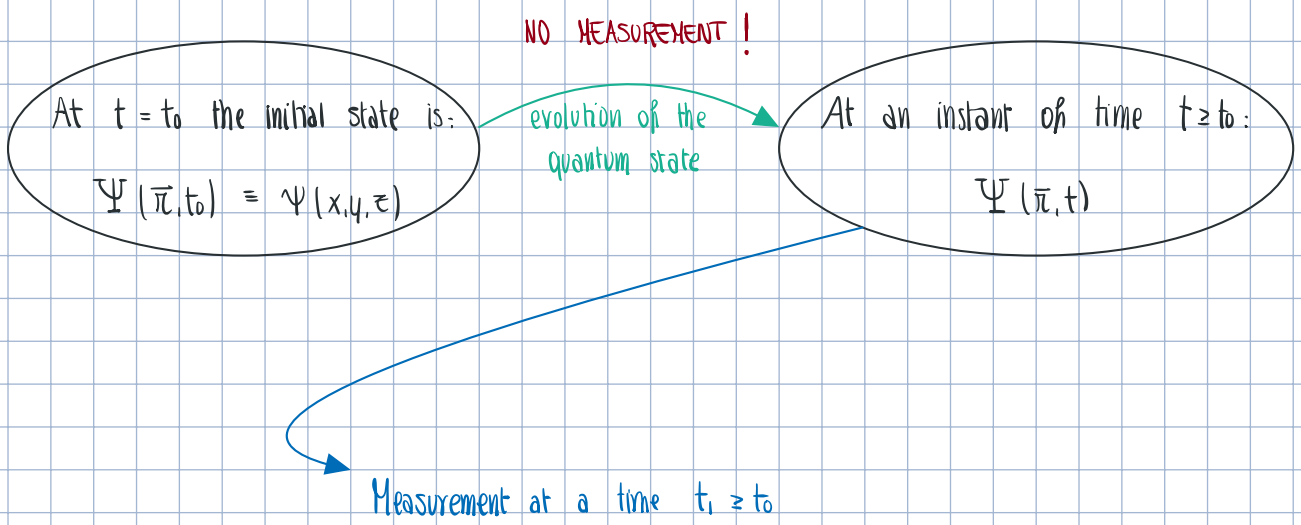
with the initial condition: $\Psi(\vec{r}_0,t_0) = \Psi(\vec{r})$, the quantum state evolution is:

$$\Psi(\vec{r},t) = e^{-\frac{i}{\hbar}(t-t_0)\hat{H}} \cdot \Psi(\vec{r},t_0)$$

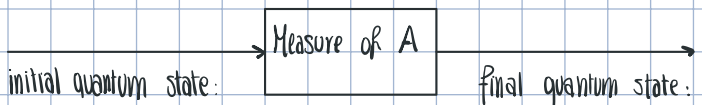
For the harmonic oscillator:

$\Psi(\vec{r},t_0) = \sum_n \lambda_n \psi_n(\vec{r})$ where $\hat{H}\psi_n(\vec{r}) = E_n \psi_n(\vec{r})$ (assuming $\hat{H}$ time-independent)

$\Psi(\vec{r},t) = \sum_n \lambda_n e^{-\frac{i}{\hbar}(t-t_0)\cdot E_n} \psi_n(\vec{r})$



We measure an observable A (a physical quantity).



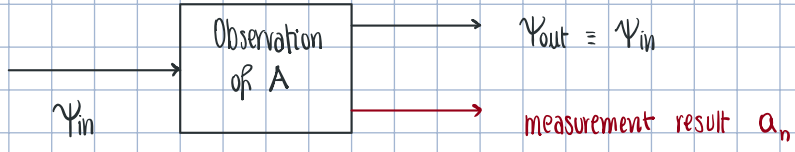
$\psi_{in}(\vec{r}) = \Psi(\vec{r}, t_1^{(-)})$ $\quad$ $\psi_{out}(\vec{r}) = \Psi(\vec{r}, t_1^{(+)})$

In general $\psi_{out}(\vec{r}) \neq \psi_{in}(\vec{r})$.

The "basic" quantum measurement is a <u>PROJECTIVE MEASUREMENT</u>: (random) collapse of the wave function into an eigenfunction of the (hermitian) operator $\hat{A}$, related to the observable A.

In case of discrete-spectrum operator:

$\hat{A}\psi_n = a_n \psi_n$ (eigenfunction for the operator $\hat{A}$)



In the Copenhagen interpretation the probability of having as a result a_n is

$P_n \propto$ scalar product between the eigenfunction ψ_n and the initial state ψ_{in}

$$\iiint_{-\infty}^{+\infty} \psi_n^*(x,y,z) \cdot \psi_{in}(x,y,z)\, dx\, dy\, dz \qquad \text{(Born's rule)}$$

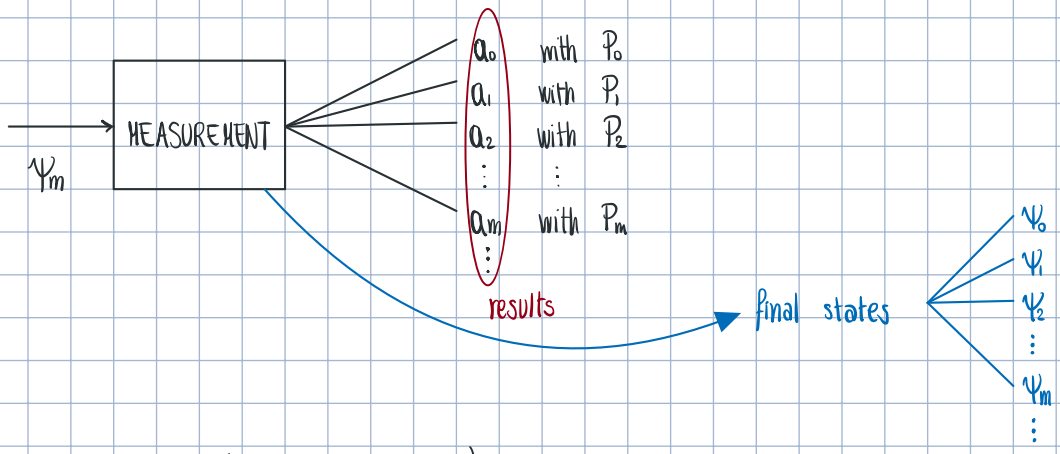
Hermitian operator $\hat{A}$.

1. eigenvalues a_n are real
2. eigenfunctions corresponding to different eigenvalues are orthogonal

$$a_m \neq a_n \implies \psi_m, \psi_n \text{ are orthogonal (i.e. null scalar product)}$$

$$\iiint_{-\infty}^{+\infty} \psi_m^* \psi_n \, dx\, dy\, dz = 0$$

If we consider $\psi_{in} \equiv \psi_n$ $(n = m)$, then the value of observable for this state it is well-defined (with no uncertainty) and equal to the eigenvalue a_n



If $\psi_{in} = \psi_m$ (m-th eigenfunction) then the probability of measuring a_n (and correspondingly to have a wave function collapse or orthogonal projection) is

$$\iiint_{-\infty}^{+\infty} \psi_m^*(x,y,z) \cdot \psi_n(x,y,z)\, dx\, dy\, dz = \delta_{mn}$$

where δ_{mn} is the Kronecker's delta:

$$\delta_{mn} = \begin{cases} 1 & \text{for } m = n \\ 0 & \text{for } m \neq n \end{cases}$$

Orthonormalization condition for eigenfunctions:

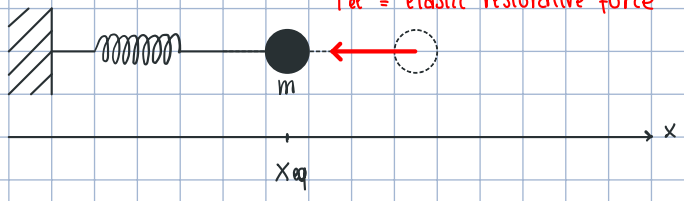
$$\iiint_{-\infty}^{+\infty} \psi_m^* \psi_m \, dx\, dy\, dz = \iiint_{-\infty}^{+\infty} |\psi_m|^2 \, dx\, dy\, dz = 1$$

This is the normalization condition, applied to the initial state $\psi_{in} = \psi_m$.

HARMONIC OSCILLATOR

Classical case

Some examples of classical harmonic oscillator can be the LC circuit or the mass attached to an elastic spring:



restoring action of the elastic force

$$F_x = -K(x - x_{eq})$$

elastic constant

At equilibrium: $F_x = 0 \quad \leftrightarrow \quad x = x_{eq}$

To write the motion equation of the system we have to use the Newton's second law:

$$\vec{F} = m\cdot\vec{a}$$

In our 1-D case:

$$F_x = m\cdot a_x \longrightarrow -K(x - x_{eq}) = m\ddot{x}$$

This is a differential equation. Putting the equilibrium point at the origin of the cartesian plane ($x_{eq} = 0$) we obtain:

$$m\cdot\frac{d^2x}{dt^2} + Kx = 0 \longrightarrow \frac{d^2x}{dt^2} + \frac{K}{m}x = 0 \xrightarrow{\omega = \sqrt{K/m}} \boxed{\frac{d^2x}{dt^2} + \omega^2 x = 0}$$

The solutions of the differential equation are:

$$\begin{cases} x(t) = A\cdot\cos(\omega t + \phi_0) \\ p(t) = m\,v_x = m\,\dot{x} = -m\omega A\cdot\sin(\omega t + \phi_0) \end{cases}$$

→ these periodic solutions give the name "harmonic" to the oscillator

We can note that $x(t)$ and $p(t)$ oscillate harmonically in QUADRATURE at the same pulsation (angular frequency) $\omega = \sqrt{K/m}$.

Imposing the initial conditions:

$$\begin{cases} x(0) = x_0 \\ p(0) = p_0 \end{cases}$$

we can determine the amplitude A, the initial phase ϕ_0 and the deterministic evolution of the system.

The kinetic energy is described by the expression:

$$E_{kin} = \frac{1}{2} m v_x^2 = \frac{p_x^2}{2m}$$

The temporal mean (average) of the kinetic energy is:

$$\overline{E_{kin}} = \frac{1}{T}\int_0^T E_{kin}(t)\,dt = \frac{1}{T}\int_0^T \frac{p_x(t)^2}{2m}\,dt = \frac{1}{T}\int_0^T \frac{m^2\omega^2A^2}{2m}\sin^2(\omega t + \phi_0)\,dt$$

period

$$= \frac{m\omega^2A^2}{2T}\cdot\frac{T}{2} = \frac{1}{4}m\omega^2A^2 = \frac{1}{4}kA^2$$

The potential energy instead, for a conservative (non-dissipating) forces is:

$$E_{pot} = V$$

$$\vec{F} = -\text{grad}\,V = -\nabla V$$

$$F_x(x) = -\frac{dV}{dx}(x)$$

$$V(x) = -\int_{x_{eq}=0}^{x} F(x')\,dx' = -\text{ work of the elastic force moving from } x_{eq} \text{ to a generic position } x.$$

$$= -\int_0^x -kx'\,dx' = k\left[\frac{x'^2}{2}\right]_0^x = \frac{kx^2}{2} = \frac{1}{2}m\omega^2x^2$$

The temporal mean of the potential energy is:

$$\overline{E_{pot}} = \frac{1}{T}\int_0^T \frac{1}{2}m\omega^2x^2(t)\,dt = \frac{1}{T}\int_0^T \frac{1}{2}m\omega^2A^2\cos^2(\omega t + \phi_0)\,dt = \frac{1}{4}m\omega^2A^2$$

$$\boxed{\overline{E_{KIN}} = \overline{E_{Pot}}}$$ for classical harmonic oscillator

The total energy (hamiltonian) is:

$$H(x, p_x) = E_{kin}(p_x) + E_{pot}(x) = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2x^2$$

Quantum mechanics

The hamiltonian, in quantum mechanics is an (hermitian) operator:

$$\hat{H} = H(\hat{x}, \hat{p}_x) = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

where $\hat{x}^2 \equiv \hat{x}^2$ and $\hat{p}_x^2 \equiv \hat{p}_x^2$

In the position-representation, where the quantum state is described by a wave function depending on the position $\Psi(x)$, we can write:

$$\begin{cases} \hat{x} \longrightarrow x \\ \hat{p}_x \longrightarrow -i\hbar \cdot \dfrac{\partial}{\partial x} \\ \hat{p}_x^2 \longrightarrow (-i\hbar)^2 \dfrac{\partial^2}{\partial x^2} = -\hbar^2 \dfrac{\partial^2}{\partial x^2} \end{cases}$$

We can write the time-independent Schrödinger's equation solutions, that are the stationary states (time-independent because in our case $\hat{H}$ is time-independent):

$$\hat{H}\Psi(x) = E\Psi(x) \qquad \text{(eigenvalue equation for } \hat{H}\text{)}$$

$$-\frac{\hbar^2}{2m}\cdot\frac{d^2}{dx^2}\Psi(x) + \frac{1}{2}m\omega^2 x^2 \cdot \Psi(x) = E\Psi(x)$$

The solutions are an infinite set of discrete:

$$\Psi_n(x) = \frac{1}{\sqrt{2^n \cdot n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \cdot \exp\left(-\frac{m\omega}{2\hbar}x\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}\cdot x\right) \qquad \text{where } n \triangleq \text{quantum number} = 0, 1, 2\ldots$$

normalization coefficient | gaussian function | Hermite polynomials of order n

$\Psi(x)$ are stationary states with well-defined energy

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

discrete values for the energy $\Rightarrow$ energy quantization!

$\Psi_n(x)$ are eigenfunctions of $\hat{H}$ with corrisponding eigenvalues E_n.

$H_0(x) = 1,$ (even)
$H_1(x) = 2x,$ (odd)
$H_2(x) = 4x^2 - 2,$ (even)
$H_3(x) = 8x^3 - 12x,$ (odd)
$H_4(x) = 16x^4 - 48x^2 + 12,$ ⋮
$H_5(x) = 32x^5 - 160x^3 + 120x,$
$H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120,$

Hermite Polynomials

$\Psi_n(x)$ have well-defined parity:

- the gaussian function is even;
- Hermite polynomials have the same parity of n.

$\Rightarrow \quad \psi_n(x)$ is $\begin{cases} \text{EVEN} & \text{for even } n \\ \text{ODD} & \text{for odd } n \end{cases}$

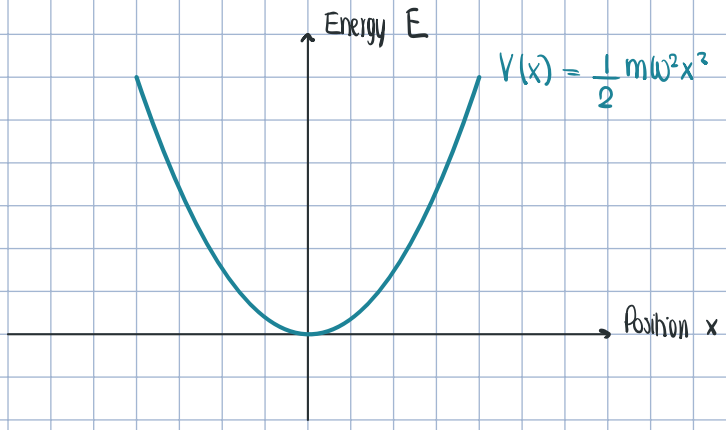
[Even: $\psi_n(-x) = \psi_n(x)$; Odd: $\psi_n(x) = -\psi_n(x)$]

The fundamental state is the minimum energy state (also called "non-exited state"). For the quantum harmonic oscillator the fundamental state is for $n = 0$:

$$\psi_0(x) = c_0 \cdot \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

and it is a gaussian wave-function!

CLASSICAL HARMONIC OSCILLATOR



Examples of harmonic oscillators are:

- resonant LC electrical circuit;
- elastic spring;
- heavy body on a cylindrical surface with periodic profile of the height.

Harmonic solutions (with period $T = \frac{2\pi}{\omega}$):

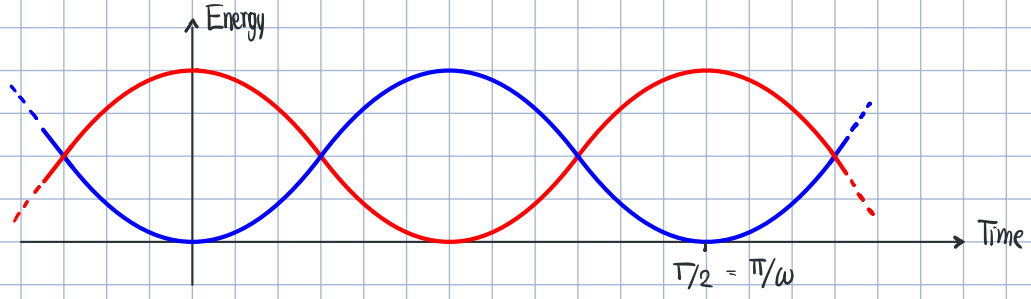
$$\begin{cases} x(t) = A\cos(\omega t + \phi_0) \\ p(t) = -Am\omega \sin(\omega t + \phi_0) \end{cases}$$

(two harmonics in quadrature)

$$\begin{cases} E_{kin} = \frac{p_x^2}{2m} = \frac{1}{2} A^2 m\omega^2 \sin^2(\omega t + \phi_0) \\ E_{pot} = \frac{1}{2} m\omega^2 x^2 = \frac{1}{2} A^2 m\omega^2 \cos^2(\omega t + \phi_0) \end{cases} \Rightarrow$$

two harmonic oscillations with period $\frac{T}{2}$ in phase opposition (or in anti-phase)

(we assume $t_0 = 0$, $\phi_0 = 0$)

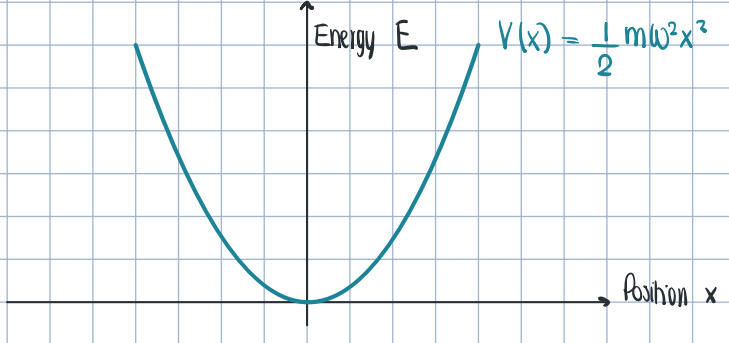


$$\overline{E_{kin}} = \overline{E_{pot}} = \frac{1}{4} A^2 m\omega^2$$

$$E_{tot}(t) = E_{kin}(t) + E_{pot}(t) = \frac{1}{2} A^2 m\omega^2 \longrightarrow$$

ENERGY CONSERVATION (assuming no dissipative forces).

QHO - QUANTUM HARMONIC OSCILLATOR



Due to the wave-particle duality and Heisenberg uncertainty principle we do not know both position and momentum with well defined value.

We start from the stationary states $\psi_n(x)$ (eigenfunctions of $\hat{H}$) with well-defined energy.

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$ (eigenvalues of $\hat{H}$) with $n = 0, 1, 2, \ldots$ (quantum number)

Energy quantization (Planck, 1901)

$$\hat{H}\psi_n = E_n\psi_n$$

In general we can say that the bounded quantum states (electron bound to an atom/ion/molecule) present discrete values of energy (energy quantization)

↕

discrete-spectrum hamiltonian $\hat{H}$ (finite or countable infinite set of eigenvalues)

and are described by finite-norm wave functions:

$$\|\psi\|^2 = \int_{-\infty}^{+\infty} \psi^*(x)\cdot\psi(x)\,dx = \int_{-\infty}^{+\infty} |\psi(x)|^2\,dx = \text{constant} \ (\neq \infty)$$

↳ squared-norm of the quantum state ψ

E.g.: normalized wave function:

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

Those finite-norm (or normalizable) wave function are elements of the function space $\mathcal{L}^2$ (which is an example of Hilbert space).

In the case of unbounded quantum states (e.g. free-particle <=> plane wave) the Hamiltonian has continuous spectrum (non-countable infinite set of eigenvalues) and the eigenfunctions are not finite-norm function. (But in any case normalizable only in generalized case).

The Hamiltonian for a free-particle:

$$\hat{H} = \frac{\hat{p}^2}{2m}$$ (zero potential energy)

Eigenfunctions of $\hat{p}^2$ and $\hat{H}$ are the same:

$$\psi(\vec{r}) = Ce^{i\vec{k}\cdot\vec{r}} = Ce^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$$

$$\psi(x,y,z) = Ce^{\frac{i}{\hbar}(p_x\cdot x + p_y y + p_z\cdot z)} = Ce^{\frac{i}{\hbar}p_x x}\,e^{\frac{i}{\hbar}p_y y}\,e^{\frac{i}{\hbar}p_z z}$$

The plane wave is eigenfunction of

$$\hat{\vec{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$$

with eigenvalues (p_x, p_y, p_z), forming a continuous set

$$-\infty < p_x, p_y, p_z < +\infty$$

Because $\hat{H}$ is function of

$$\hat{p}^2 = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2$$

$$\Downarrow$$

The eigenvalue of $\hat{H}$ for the plane wave eigenfunction is:

$$E = \frac{p^2}{2m} = \frac{p_x^2 + p_y^2 + p_z^2}{2m} \longrightarrow -\infty < E < +\infty \quad \text{(assuming all real values)}$$

$\Rightarrow$ no quantization for the free particle!

The plane wave eigenfunction of $\hat{H}$ for free particle has infinite norm:

$$\| e^{i\vec{k}\cdot\vec{r}} \|^2 = \iiint_{-\infty}^{+\infty} \left(e^{i\vec{k}\cdot\vec{r}}\right)^* \cdot e^{i\vec{k}\cdot\vec{r}}\, dx\, dy\, dz = \iiint_{-\infty}^{+\infty} \underbrace{e^{-i\vec{k}\cdot\vec{r}} \cdot e^{i\vec{k}\cdot\vec{r}}}_{=1} dx\, dy\, dz = \infty$$

$\Rightarrow$ the plane wave is completely delocalized:

$$P(\vec{r}) = |\psi(x,y,z)|^2 = |e^{i\vec{k}\cdot\vec{r}}| = 1$$

↳ probability density function of "localizing" in $\vec{r}(x,y,z)$ (measuring the position of the particle)

Completely delocalized states	$\longleftrightarrow$	Infinit-norm $\psi(x,y,z)$
(Partially) Delocalized states	$\longleftrightarrow$	Finite-norm $\psi(x,y,z)$ (normalizable)
Continuous-spectrum $\hat{H}$ (time independent)	$\longleftrightarrow$	Infinite-norm ψ_x stationary states (eigenfunctions) forming a continuous infinite set
Discrete-spetrum $\hat{H}$ (time-independent)	$\longleftrightarrow$	Normalizable stationary states (eigenfunctions) ψ_n forming a discrete set (finite or infinite).

The fundamental state of a QHO is described by a Gaussian wave function:

$$\psi_0(x) = C \cdot e^{-\frac{m\omega}{2\hbar}x^2}$$ where $\sqrt{\frac{2\hbar}{m\omega}}$ is a characteristic length of a quantum oscillator.

$$P(x) = |\psi_0(x)|^2 = |C|^2 \cdot e^{-\frac{m\omega}{\hbar}x^2} \propto e^{-\frac{x^2}{2\sigma_x^2}}$$ gaussian distribution for the probability of position measurement

$\sigma_x^2 = \frac{\hbar}{2m\omega}$ variance in the position measurement

The uncertainty in the position measurement is:

$$\Delta x = \sigma_x = \sqrt{\frac{\hbar}{2m\omega}}$$

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \frac{\hbar\omega}{2}\left(\hat{\xi}^2 + \hat{\eta}^2\right)$$

adimensional observables (hermitian operators)

$$\begin{cases} \hat{\xi} = \sqrt{\frac{1}{m\hbar\omega}}\,\hat{p}_x \\ \hat{\eta} = \sqrt{\frac{m\omega}{\hbar}}\,\hat{x} \end{cases}$$

The momentum uncertainty and the position uncertainty for ψ_0 are:

$$\Delta p_x = \sqrt{\frac{m\omega\hbar}{2}} \qquad \Delta x = \sqrt{\frac{\hbar}{2m\omega}}$$

For the fundamental state of QHO:

$$\Delta x \cdot \Delta p_x = \frac{\hbar}{2}$$ The gaussian wave function ψ_0 is a minimum uncertainty wave function

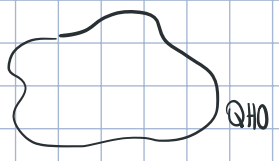
In general, for any ψ of any quantum system:

$$\Delta x \cdot \Delta p_x \geq \frac{\hbar}{2}$$ HEISENBERG'S UNCERTAINTY PRINCIPLE

For the fundamental state of the harmonic oscillator, the product between the uncertainties of the "canonically conjugate" observable position x and momentum p_x is equal to the minimum $\frac{\hbar}{2}$ predicted by uncertainty principle.

QUANTUM HARMONIC OSCILLATOR (QHO)

Quantum state Ψ of QHO is identified by a ray of the Hilbert space $\mathcal{H}$



$\longleftrightarrow$ $\mathcal{H}$

quantum state $\longleftrightarrow$ $|\psi\rangle$ (apart a nonzero multiplicative complex scalar γ).

$\longleftrightarrow$ $\langle\psi| = |\psi\rangle^\dagger$

$\gamma|\psi\rangle$ and $|\psi\rangle$ describe the same quantum state. We know $F(\gamma\psi, \psi) = 1$

We can choose a normalized Ket $|\psi\rangle$ for describing the quantum state (anyway there is a phase ambiguity).

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

$\| \gamma|\psi\rangle \|^2$ = scalar product between $\gamma|\psi\rangle$ and $\gamma|\psi\rangle = (\gamma|\psi\rangle)^\dagger \cdot \gamma|\psi\rangle$

$$= \gamma^* |\psi\rangle^\dagger \cdot \gamma|\psi\rangle = \gamma^* \langle\psi| \cdot \gamma|\psi\rangle = \gamma^*\gamma \langle\psi|\psi\rangle$$

$$= |\gamma|^2 \langle\psi|\psi\rangle$$

For example, if $|\psi\rangle$ is normalized:

$$\|\psi\|^2 = \langle\psi|\psi\rangle = 1$$

but if we have $\gamma = e^{i\delta}$, then

$$\|\gamma\psi\|^2 = |\gamma|^2 \|\psi\|^2 = |\gamma|^2 = 1$$

If $|\psi\rangle$ is a normalized Ket, then also $e^{i\delta}|\psi\rangle$ is a normalized Ket.

Energy representation

The orthonormal basis $\{ |\psi_n\rangle, n = 0, 1, 2, \dots \}$ of the Hilbert space of Kets is given by the eigenKets (eigenvector) of the hamiltonian operator (energy observable)

$$\hat{H}|\psi_n\rangle = E_n |\psi_n\rangle$$

The eigenvalues E_n are the possible results of energy measurement.

Time-dependent Schrödinger's equation $\Rightarrow$ $|\psi_n\rangle$ are the stationary quantum states for the QHO (states with well defined energy E_n).

A generic quantum state can be expanded as:

$$|\psi\rangle = \sum_{n=0}^{\infty} \lambda_n |\psi_n\rangle$$

with scalar coefficients:

$$\lambda_n = \langle \psi | \psi_n \rangle$$

$$\downarrow$$

$$\begin{bmatrix} \lambda_0 = \langle \psi | \psi_0 \rangle \\ \lambda_1 = \langle \psi | \psi_1 \rangle \\ \lambda_2 = \langle \psi | \psi_2 \rangle \\ \vdots \\ \lambda_n = \langle \psi | \psi_n \rangle \end{bmatrix}$$

column vector representing $|\psi\rangle$

$$|\psi\rangle \longleftrightarrow \begin{bmatrix} \lambda_0 \\ \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \end{bmatrix}$$

$|\psi\rangle$: Ket

Hilbert space ($\mathcal{H}$)

duality

$$|\psi\rangle^{\dagger} = \langle \psi | \longleftrightarrow \begin{bmatrix} \lambda_0^* & \lambda_1^* & \dots & \lambda_n^* \end{bmatrix}$$

$\langle \psi |$: bra

Dual Hilbert space ($\mathcal{H}^*$)

"$\dagger$": DAGGER: in terms of matrix algebra is the hermitian conjugated (conjugated ↓ complex conjugation: $*$ transposed) ↓ transposition: exchange between raws and columns

Position representation

The position operator $(\hat{x}, \hat{y}, \hat{z})$ is a continuous-spectrum hermitian operator.

(no quantization/discretization in the position measurament)

The eigenvalues form a continuum (non-countable infinite set)

$-\infty < x, y, z < +\infty$

(any real value is a possible result of the measurement of x, y, z). Also the eigenkets form a continuum! We can identify the eigenkets of $\hat{x}$ with eigenvalues x' as the Dirac's delta functions, centered in x':

$\delta(x-x')$ (continuous spectrum $\Rightarrow$ infinite norm eigenkets)

$$\| \delta(x-x') \|^2 = \int_{-\infty}^{+\infty} \delta(x-x') \cdot \overline{\delta(x-x')}^{\,x=x'} \, dx$$

We know that:

$$\int_{-\infty}^{+\infty} \delta(x-x') \cdot f(x) \, dx = f(x')$$

$$\| \delta(x-x') \|^2 = \delta(0) \longrightarrow +\infty$$

Generalized orthonormalization condition (for eigenkets of continuous-spectrum observables)

$$\int_{-\infty}^{+\infty} \delta(x-x') \cdot \delta(x-x'') \, dx = \delta(x'-x'')$$

$\delta(x-x') \longleftrightarrow |\psi_{x'}\rangle = |x'\rangle$ eigenket of $\hat{x}$ with eigenvalue x'

$$\hat{x}\,|x'\rangle = x'\,|x'\rangle$$

$$\langle x'|x''\rangle = \delta(x'-x'') = \begin{cases} \infty & \text{for } x' = x'' \\ 0 & \text{for } x' \neq x'' \end{cases}$$

The wave function $\psi(x)$ is the representation of $|\psi\rangle$ considering the eigenkets of the position operator $\hat{x}$ as orthonormalized basis (in the generalized sense)

The ket $|\psi\rangle$ is "expanded" in terms of the basis kets $|x\rangle$ with "coefficients":

$$\langle x|\psi\rangle = \int_{-\infty}^{+\infty} \delta^*(\xi - x) \cdot \psi(\xi) \, d\xi = \psi(x)$$

$f(\xi)$ evaluated in $\xi = x$

Born's rule: the probability density function of measuring a position x is given by

$$\mathcal{P}(x) = |\langle x|\psi\rangle|^2 = \left| \int_{-\infty}^{+\infty} \delta^*(\xi - x) \cdot \psi(\xi) \, d\xi \right|^2 = |\psi(x)|^2$$

For the harmonic oscillator and in general for any quantum-mechanical system with bounded states, the hamiltonian $\hat{H}$ has discrete spectrum (energy quantization).

We can represent any quantum state described by a ket $|\Psi\rangle$ as discrete superposition of the basis kets

$$\{ |\Psi_n\rangle \quad \text{with non-negative integer} \quad n = 0, 1, 2, \dots \}$$

which are orthonormalized elements of $\hat{H}$:

$$\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle \qquad \text{(time-independent Schrödinger's equation)}$$

that is $|\Psi_n\rangle$ describes the quantum state having well-defined value of energy E_n (eigenvalues of $\hat{H}$). If $\hat{H}$ is time-independent then $|\Psi_n\rangle$ are stationary states.

Orthonormalization condition for the basis:

$$\langle \Psi_m | \Psi_n \rangle = \delta_{mn}$$

$$|\Psi\rangle = \sum_{n=0}^{\infty} \lambda_n |\Psi_n\rangle \qquad \text{for any } |\Psi\rangle \qquad \text{(completeness of Hilbert space)}$$

λ_n: scalar complex coefficients of the superposition

$$\lambda_n = \langle \Psi_n | \Psi \rangle$$

Example: demonstrate this expression for λ_n using Dirac's notation.

For the completeness of Hilbert space:

$$|\Psi\rangle = \sum_n \lambda_n |\Psi_n\rangle$$

for the linearity of the scalar product in the second term

$$\langle \Psi_n | \Psi \rangle = \langle \Psi_n | \sum_m \lambda |\Psi_m\rangle = \sum_n \lambda_n \langle \Psi_n | \Psi_m \rangle$$

δ_{nm}, orthonormalization condition

$$= \sum_m \lambda_n \delta_{mn} = \lambda_n \delta_{nn} = \lambda_n \cdot 1 = \lambda_n$$

for $m = n$

For qubits we have just $n = 0, 1$!

The superposition can be written as:

$$|\psi\rangle = \sum_n \lambda_n |\psi_n\rangle = \sum_n \langle\psi_n|\psi\rangle |\psi_n\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\psi\rangle = \hat{1}|\psi\rangle$$

identity operator

$$\sum_{n=0}^{+\infty} |\psi_n\rangle\langle\psi_n| = \hat{1}$$ CLOSURE PROPERTY (with $\{|\psi_n\rangle;\ n = 0, 1, 2, \ldots\}$ forming an orthonormalized basis)

The closure property is related to the completeness and orthonormalization of $\{|\psi_n\rangle\}$

A possible choise of the basis $\{|\psi_n\rangle\}$ is given by the eigenkets of $\hat{H}$ (energy observable)

(energy representation)

But in general, we can choose an orthonormal basis of the Hilbert space describing the quantum system formed by the eigenkets of any hermitian operator (i.e. observables).

Position representation

In the position representation, the basis of Hilbert space is formed by eigenstates of the position operator $\hat{x}$ (x component of position)

→ continuous-spectrum operator

$\hat{x}$ has a non-countable infinite set (a "continuum") of eigenvalues $-\infty < x < +\infty$:

$$\hat{x}|x\rangle = x|x\rangle$$ eigenvalue equation for the operator $\hat{x}$

$\hat{x}$: hermitian operator; $|x\rangle$: eigenkets; x: real eigenvalue (result of position measurement)

Continuous basis:

$$\{|x\rangle \text{ with } x \in \mathbb{R}\}$$ (any real value x)

Generalized orthonormalization condition: if $|x'\rangle$ and $|x''\rangle$ are two eigenkets of $\hat{x}$, then

$$\langle x'|x''\rangle = \delta(x'-x'') = \begin{cases} \infty & \text{for } x' = x'' \\ 0 & \text{for } x' \neq x'' \end{cases}$$

Continuous expansion (quantum superposition principle in the continuous case)

$$|\psi\rangle = \int_{-\infty}^{+\infty} \lambda_x |x\rangle\, dx$$

λ_x: complex function of x

for the completeness of Hilber space and the completeness of $\{|x\rangle\}$ basis

$\lambda_x = \langle x|\psi\rangle = \psi(x)$ wave function in the position representation

E.g.: $\langle x|\psi\rangle = \langle x| \int_{-\infty}^{+\infty} \lambda_\xi |\xi\rangle \, d\xi$ for the linearity of the scalar product in the second element

$= \int_{-\infty}^{+\infty} \lambda_\xi \langle x|\xi\rangle \, d\xi$

$= \int_{-\infty}^{+\infty} \lambda_\xi \, \delta(x-\xi) \, d\xi = \lambda_x$

function evaluated at the center of Dirac's delta, i.e. $\xi = x$

For the Born's rule the probability density function of measuring a value (eigenvalue) x for position is:

$$P(x) = |\langle x|\psi\rangle|^2 = |\psi(x)|^2$$

We can identify

$$\psi(x) = \langle x|\psi\rangle = \lambda_x$$

In case of energy representation, the Born's rule says that the probability of measuring En in case of initial ket $|\psi\rangle$ is equal to: quantum state collapse in $|\psi_n\rangle$ due to the energy measurement

$$P_n = F(\psi, \psi_n) = |\langle \psi_n|\psi\rangle|^2$$

↓ fidelity between the ket $|\psi\rangle$ before the measurement and the eigenket $|\psi_n\rangle$

In the position representation we can write:

$$|\psi\rangle = \int_{-\infty}^{+\infty} |x\rangle \langle x|\psi\rangle \, dx$$

$\langle x|\psi\rangle$: wave function

The closure property in continuous case is:

$$\int_{-\infty}^{+\infty} |x\rangle\langle x| \, dx = \hat{I}$$

The wave functions of the eigenKets of the position operator $\hat{x}$ are Dirac's delta centered in the eigenvalue.

Demonstration:

- Hyp.: $|x'\rangle$ eigenket of $\hat{x}$

$$x|x'\rangle = x'|x'\rangle$$

- Th.: $\psi_{x'}(x) = \delta(x-x')$

$$|\psi\rangle = \hat{1}\,|\psi\rangle = \int_{-\infty}^{+\infty} |x\rangle\langle x|\psi\rangle\, dx$$

($\hat{1}$: identity operator; the integral: for the closure property)

for any ket $|\psi\rangle$. In particular we consider:

$$|\psi\rangle = |x'\rangle$$

wavefunction $\psi_{x'}(x)$ for the eigenket $\Rightarrow$ eigenfunction of $\hat{x}$

$$|x'\rangle = \int_{-\infty}^{+\infty} |x\rangle\langle x|x'\rangle\, dx$$

For the generalized orthonormalized condition:

$$\psi_{x'}(x) = \langle x|x'\rangle = \delta(x-x')$$

We can write the completeness property in terms of wave functions as continuous expansion in the position representation

$$\psi(x) = \int_{-\infty}^{+\infty} \psi(\xi)\,\delta(x-\xi)\,d\xi$$

Property of Dirac's delta:

Demonstration:

$$|\psi\rangle = \int |\xi\rangle\langle\xi|\psi\rangle\, d\xi$$

$$\langle x|\psi\rangle = \int \underbrace{\langle x|\xi\rangle}_{\delta(x-\xi)}\underbrace{\langle\xi|\psi\rangle}_{\psi(\xi)}\, d\xi$$

$$\psi(x) = \int \psi(\xi)\,\delta(x-\xi)\,d\xi$$

$\hat{x}$ operator in position representation $\Longleftrightarrow$ (hermitian) operator with eigenfunction $\delta(x-x')$ and eigenvalues x' $\Longleftrightarrow$ multiplication of the wave function $\psi(x)$ by x.

Born's rule in position representation for measuring the position in case of an eigenfunction of position:

$$\mathcal{P}(x') = F(x', x) = |\langle x|x'\rangle|^2 = |\psi'(x)|^2 = |\delta(x-x')|^2$$

↳ probability density function of measuring a position x'.

For position eigenfunction:

$$\mathcal{P}(x') = \begin{cases} \infty & \text{for } x = x' \\ 0 & \text{for } x \neq x' \end{cases}$$

⇓

"Completely sharp" localization of the particle.

MOMENTUM REPRESENTATION

The momentum (x-component) operator $\hat{p}_x$ is a continuous spectrum operator (canonically conjugated to position):

$$\hat{p}_x |p_x\rangle = p_x |p_x\rangle$$

(hermitian) momentum operator — eigenket of $\hat{p}_x$ (quantum state with well-defined momentum p_x) — real eigenvalue

Continuous basis of the Hilbert space: $\{|p_x\rangle$ with any $p_x \in \mathbb{R}\}$

$$\langle p_x' | p_x'' \rangle = \delta(p_x' - p_x'')$$

Closure property:

$$\int_{-\infty}^{+\infty} |p_x\rangle\langle p_x| \, dp_x = \hat{1}$$

Expansion in $\{|p_x\rangle\}$ eigenket basis:

$$|\psi\rangle = \hat{1}|\psi\rangle = \int_{-\infty}^{+\infty} |p_x\rangle \langle p_x|\psi\rangle \, dp_x$$

$\langle p_x|\psi\rangle$: Wave function in the momentum representation (scalar product between an eigenstate of the momentum by the considered quantum state ψ).

$$\tilde{\psi}(p_x) = \langle p_x|\psi\rangle$$

It is possible to demonstrate:

$$\tilde{\Psi}(p_x) = \frac{1}{\sqrt{h}} \mathcal{F}\{\Psi(x)\}\Big|_{f_x = \frac{\omega_x}{2\pi} = \frac{p_x}{h}}$$

De-Broglie relation:

$$p_x = \hbar K_x = \frac{h}{2\pi} \omega_x$$

DIRECT DOMAIN	FOURIER (or reciprocal) DOMAIN
time t	frequency f [1/time]
spatial coordinate x	x-component of spatial frequency f_x [1/length]
" " y	" " f_y
" " z	" " f_z

$$\begin{cases} f = \frac{1}{T} = \frac{\omega}{2\pi} \\ f_x = \frac{1}{\lambda} = \frac{K_x}{2\pi} \end{cases} \qquad \left(K = \frac{2\pi}{\lambda}\right)$$

Fourier transform:

$$\mathcal{F}\{\Psi(x)\} = \int_{-\infty}^{+\infty} \Psi(x) \cdot e^{-2\pi i f_x x} \, dx$$

$$\tilde{\Psi}(p_x) = \frac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} \Psi(x) \cdot e^{-i \frac{2\pi}{h} p_x \cdot x} \, dx = \frac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} \Psi(x) \cdot e^{-\frac{i}{\hbar} p_x \cdot x} \, dx$$

($1/\hbar$)

Fourier transform of identity:

$\Psi(x) = 1$ for any real x is the Dirac's delta:

$$\mathcal{F}\{1\} = \int_{-\infty}^{+\infty} e^{-2\pi i f_x \cdot x} \, dx = \delta(f_x)$$

Fourier transform extended to tempered distribution

Integral as "principal value"

"generalized" function (tempered distribution)

The eigenstates of the momentum (according to the diffraction and interference experiments) are described by "plane-waves" wave functions:

$$\psi_{p_x}(x) = C e^{ik_x x} = C e^{i\frac{p_x}{\hbar}x} \qquad \text{(with any complex constant } C \neq 0\text{)}$$

↳ infinite norm (the squared module $|\psi_{p_x}(x)|^2$ is not integrable: $\int_{-\infty}^{+\infty} |\psi_{p_x}(x)|^2 dx = |c|^2 \int_{-\infty}^{+\infty} dx = +\infty$)

For the generalized orthonormalization of the basis $\{|p_x\rangle\}$ we have $C = \frac{1}{\sqrt{h}} = h^{-1/2}$

$$\langle p_x' | p_x'' \rangle = \delta(p_x' - p_x'')$$

in position representation

Demonstration: $\psi_{p'x}$

$$\int_{-\infty}^{+\infty} \psi'(x)^* \cdot \psi''(x)\, dx = \int_{-\infty}^{+\infty} \left(\frac{1}{\sqrt{h}} e^{i\frac{p_x'}{\hbar}x}\right)^* \cdot \frac{1}{\sqrt{h}} e^{i\frac{p_x''}{\hbar}x} dx$$

$$= \frac{1}{h}\int_{-\infty}^{+\infty} e^{-i\frac{p_x'}{\hbar}x} \cdot e^{i\frac{p_x''}{\hbar}x} dx = \frac{1}{h}\int_{-\infty}^{+\infty} 1 \cdot e^{-i\frac{2\pi}{h}(p_x' - p_x'')x} dx$$

Fourier transform Kernel with $f_x = (p_x' - p_x'')\,h$

$$= \frac{1}{h} F\{1\}\Big|_{f_x = \frac{p_x' - p_x''}{h}} = \frac{1}{h}\delta\left(\frac{p_x' - p_x''}{h}\right)$$

$$= \frac{1}{h} \cdot h\, \delta(p_x' - p_x'') = \delta(p_x' - p_x'') \qquad \left[\delta\left(\frac{\xi}{a}\right) = |a|\,\delta(\xi)\right]$$

We have verified:

$$\langle p_x' | p_x'' \rangle = \delta(p_x' - p_x'')$$

Now we want to demonstrate that the wave function $\tilde{\psi}(p_x)$ is (apart a coefficient) a suitable scaled Fourier transform of $\psi(x)$

$$\tilde{\psi}(p_x) = \langle p_x | \psi \rangle = \langle p_x | \hat{I} | \psi \rangle = \langle p_x \Big| \int_{-\infty}^{+\infty} |x\rangle\langle x|\, dx \,\Big| \psi \rangle$$

$$= \left\langle p_x \Big| \int_{-\infty}^{+\infty} |x\rangle\langle x|\psi\rangle\, dx \right\rangle = \int_{-\infty}^{+\infty} \langle p_x | x \rangle \langle x | \psi \rangle\, dx$$

$$= \int_{-\infty}^{+\infty} \psi(x) \cdot \langle x | p_x \rangle^*\, dx$$

scalar product between a position eigenstate and the considered state $\psi \Rightarrow \psi(x)$

$\langle x | p_x \rangle$ is the eigenfunction of p_x in the position representation:

$$\langle x|p_x\rangle = \psi_{p_x}(x) = \frac{1}{\sqrt{h}} e^{i\frac{p_x}{\hbar}\cdot x} = \frac{1}{\sqrt{h}} e^{i\cdot\frac{2\pi}{h}p_x\cdot x}$$

$$\tilde{\psi}(p_x) = \frac{1}{\sqrt{h}}\int_{-\infty}^{+\infty} \psi(x)\cdot e^{-i\frac{2\pi}{h}p_x\cdot x}\,dx = \frac{1}{\sqrt{h}}\,\mathcal{F}\{\psi(x)\}\Big|_{f_x=\frac{p_x}{h}}$$

$\hat{p}_x$ operator in position representation $\Leftrightarrow$ (hermitian) operator with eigenfunctions $\frac{1}{\sqrt{h}} e^{i\frac{p_x'}{\hbar}x}$ and eigenvalues p_x'

$\Updownarrow$

Derivative of wave functions $\psi(x)$:

$$-i\hbar\frac{d}{dx}$$

Demonstration:

$$-i\hbar\frac{d}{dx}\left(e^{i\frac{p_x'}{\hbar}x}\right) = -i\hbar\left(i\cdot\frac{p_x'}{\hbar}\right)\cdot\left(e^{i\frac{p_x'}{\hbar}x}\right) = p_x'\cdot e^{i\frac{p_x'}{\hbar}x}$$

ABSTRACT HILBERT SPACE	POSITION REPRESENTATION	MOMENTUM REPRESENTATION
quantum state $\|\psi\rangle$	$\psi(x) = \langle x\|\psi\rangle$ position-dependent wave function	$\tilde{\psi}(p_x) = \langle p_x\|\psi\rangle$ momentum-dependent wave function

Eigenstate of $\hat{x}$: $|x'\rangle$ — eigenfunction $\delta(x-x') = \langle x|x'\rangle \xrightarrow{\mathcal{F}} \frac{1}{\sqrt{h}} e^{-i\frac{p_x x'}{\hbar}}$

Eigenstate of $\hat{p}_x$: $|p_x'\rangle$ — $\frac{1}{\sqrt{h}} e^{i\frac{p_x'}{\hbar}x} \xrightarrow{\mathcal{F}} \delta(p_x-p_x')$

Action of op. $\hat{x}$: $\hat{x}|\psi\rangle$ — $x\cdot\psi(x)$ — $i\hbar\frac{d}{dp_x}\tilde{\psi}(p_x)$

Action of op. $\hat{p}_x$: $\hat{p}_x|\psi\rangle$ — $-i\hbar\frac{d}{dx}\psi(x)$ — $p_x\cdot\tilde{\psi}(p_x)$

EXPECTATION VALUE (of an observable A)

quantum (projective) measurement of an observable $\Longleftrightarrow$ random and irreversible collapse (or projection) of the quantum state into an eigenstate of $\hat{A}$ with probability given by the Born's rule:

$$P_n = F(\psi, \varphi_n) = \frac{|\langle\varphi_n|\psi\rangle|^2}{\langle\varphi_n|\varphi_n\rangle\langle\psi|\psi\rangle}$$

FIDELITY between "initial" and "final" states

(Squared modulus of scalar product between normalized vectors)

Expectation value of an observable A $\stackrel{def}{=}$ statistical mean of the results of measurement of A

Observable A $\longleftrightarrow$ random variable A that can assume the values a_n with probabilities P_n respectively.

Statistical (or "ensemble") mean:

$$\mathbb{E}(A) \equiv \langle A \rangle$$

$\mathbb{E}(A)$: random variable

$\langle A \rangle$: quantum expression in the Dirac's notation

$$\mathbb{E}(A) = \sum_n a_n P_n$$

So we can write:

$$\langle A \rangle_\psi = \sum_n a_n P_n = \sum_n a_n |\langle\varphi_n|\psi\rangle|^2$$

(assuming normalized kets $|\varphi_n\rangle$ and $|\psi\rangle$)

The expectation value $\langle A \rangle$ depends on the initial state Ψ !

We can write also :

$$\langle A \rangle_\Psi = \frac{\langle \Psi | \hat{A} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

operator $\hat{A}$ applied to the initial Ket $|\Psi\rangle$

For normalized Ket $|\Psi\rangle$:

$$\boxed{\langle A \rangle_\Psi = \langle \Psi | \hat{A} | \Psi \rangle}$$

EXERCISE : demonstrate the previous expression taking into account the statistical definition of the expectation value.

SOLUTION : We expand $|\Psi\rangle$ in the orthonormal basis $\{ |\varphi_n\rangle$, with $n = 0, 1, 2, \dots \}$ formed by the eigenkets of the hermitian operator $\hat{A}$.

$$|\Psi\rangle = \hat{1} |\Psi\rangle = \sum_n |\varphi_n\rangle \langle \varphi_n | \Psi \rangle = \sum_n \lambda_n |\varphi_n\rangle$$

$\hat{1}$: identity operator in the Kets space

$\sum_n |\varphi_n\rangle \langle \varphi_n|$: closure property

$\lambda_n |\varphi_n\rangle$ is the n-th complex (scalar) coefficient of the expansion (scalar projection of the normalized $|\Psi\rangle$ on the normalized basis eigenket $|\varphi_n\rangle$).

We write also the expansion of the bra $\langle \Psi |$:

$$\langle \Psi | = |\Psi\rangle^+ = \left(\sum_m \lambda_m |\varphi_m\rangle \right)^+ = \sum_m \lambda_m^* |\varphi_m\rangle^+ = \sum_m \lambda_m^* \langle \varphi_m |$$

$\langle \varphi_m |$: eigenbra of $\hat{A}$

$$\left(\sum_m \lambda_m |\varphi_m\rangle \right)^+ = \sum_m |\varphi_m\rangle^+ \lambda_m^+ = \sum_m \langle \varphi_m | \lambda_m^* = \sum_m \lambda_m^* \langle \varphi_m |$$

$$\begin{cases} \lambda_m = \langle \varphi_m | \Psi \rangle \\ \lambda_m^* = \langle \varphi_m | \Psi \rangle^* = \langle \Psi | \varphi_m \rangle \end{cases}$$

$$\langle \Psi | = \sum_m \langle \Psi | \varphi_m \rangle \langle \varphi_m |$$

$\sum_m \langle \Psi | \varphi_m \rangle \langle \varphi_m |$: closure property

$$\langle \Psi | = \langle \Psi | \hat{1}$$

$\hat{1}$: identity operator in the bra space

$\hat{1}|\cdot\rangle$: identity operator in the Hilbert space $\mathcal{H}$ of Kets (so acting on Kets from left-side).

$\langle\cdot|\hat{1}$: dual identity operator in dual Hilbert space $\mathcal{H}^*$ of bras (so acting on bras from right-side).

The identity operator $\hat{1}$ has the same formal expression in Dirac's notation in both "direct" $\mathcal{H}$ and "dual" $\mathcal{H}^*$:

$$\hat{1}|\cdot\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\cdot\rangle$$

$$\langle\cdot|\hat{1}^\dagger = \sum_n \langle\cdot|\varphi_n\rangle\langle\varphi_n| \qquad \text{but } \hat{1}^\dagger = \hat{1}$$

This happens for all and only the hermitian operators!

The hermitian operators are the linear self-adjoint operators:

$$\hat{A}^\dagger = \hat{A} \qquad (\text{adjoint operator: } \hat{A}^{(adj)} \equiv \hat{A}^\dagger)$$

Also the duality operation is expressed by the symbol "†".

If we only consider the operator $\hat{A}|\cdot\rangle$, then the dual operator is:

$$\langle\psi|\hat{A}^{(dual)} = \left(\hat{A}|\psi\rangle\right)^{(dual)} = \left(\hat{A}|\psi\rangle\right)^\dagger = |\psi\rangle^\dagger\cdot\hat{A}^\dagger = \langle\psi|\hat{A}^\dagger = \langle\psi|\hat{A}^{(dual)}$$

↳ final bra obtained applying $\hat{A}^{(dual)}$ to an initial bra

For hermitian operators:

$$\hat{A}^\dagger = \hat{A}$$

For example: $\hat{1} \equiv \sum_n |\varphi_n\rangle\langle\varphi_n|$

$$\begin{cases} \hat{1}|\cdot\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\cdot\rangle \\ \langle\cdot|\hat{1} = \sum_n \langle\cdot|\varphi_n\rangle\langle\varphi_n| \end{cases} \quad \dagger \quad (\dagger)$$

$$\left(\sum_n |\varphi_n\rangle\langle\varphi_n|\cdot\rangle\right)^\dagger = \sum_n \langle\varphi_n|\cdot\rangle^\dagger\cdot|\varphi_n\rangle^\dagger = \sum_n \langle\varphi_n|\cdot\rangle^*\cdot\langle\varphi_n|$$

$$= \sum_n \langle\cdot|\varphi_n\rangle\langle\varphi_n|$$

So:

$$\langle A \rangle_\psi = \langle \psi | \hat{A} | \psi \rangle = \sum_m \langle \psi | \varphi_m \rangle \langle \varphi_m | \hat{A} | \sum_n | \varphi_n \rangle \langle \varphi_n | \psi \rangle =$$

$$= \sum_m \langle \psi | \varphi_m \rangle \langle \varphi_m | \sum_n \hat{A} | \varphi_n \rangle \langle \varphi_n | \psi \rangle$$

linear hermitian operator

But:

$$\hat{A} | \varphi_n \rangle = a_n | \varphi_n \rangle$$

[real] eigenvalue of $\hat{A}$

$$\langle A \rangle_\psi = \sum_m \langle \psi | \varphi_m \rangle \langle \varphi_m | \sum_n a_n | \varphi_n \rangle \langle \varphi_n | \psi \rangle$$

$$= \sum_m \langle \psi | \varphi_m \rangle \sum_n a_n \langle \varphi_m | \varphi_n \rangle \langle \varphi_n | \psi \rangle$$

for the linearity of the scalar product in the second element

$$= \sum_m \sum_n \langle \psi | \varphi_m \rangle a_n \langle \varphi_m | \varphi_n \rangle \langle \varphi_n | \psi \rangle$$

for the orthonormalization of the eigenket basis: $= \delta_{mn}$ → Kronecker's delta

$$= \sum_m \sum_n a_n \langle \psi | \varphi_m \rangle \delta_{mn} \langle \varphi_n | \psi \rangle$$

where δ_{mn} is the Kronecker's Delta:

$$\delta_{mn} = \begin{cases} 1 & \text{for } m = n \\ 0 & \text{for } m \neq n \end{cases}$$

To conclude:

$$\langle A \rangle_\psi = \sum_{m=n} a_m \langle \psi | \varphi_m \rangle \langle \varphi_m | \psi \rangle = \sum_m a_m \langle \varphi_m | \psi \rangle^* \langle \varphi_m | \psi \rangle$$

$$= \sum_m a_m | \langle \varphi_m | \psi \rangle |^2$$

$$\boxed{= \sum_m a_m p_m}$$

We can define the uncertainty ΔA of an observable A as the standard deviation (i.e. the square root of the variance) of the results of the measurement of A.

observable A ⟷ hermitian operator $\hat{A}$ ⟷ random variable A

If we consider the random variable A:

$$\text{variance of } A = \mathbb{E}\left(A - \mathbb{E}(A) \right)^2$$

We can write this expression in quantum formalism:

$$\text{var}(A) = (\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle$$

For the linearity of mean (expectation value) with respect to A:

$$\text{var}(A) = \langle A^2 - 2\langle A \rangle A + \langle A \rangle^2 \rangle = \langle A^2 \rangle - 2\langle A \rangle \langle A \rangle + \langle A \rangle^2$$

$$= \langle A^2 \rangle - 2\langle A \rangle^2 + \langle A \rangle^2$$

$$= \langle A^2 \rangle - \langle A \rangle^2$$

Standard deviation of A (uncertainty of the observable A):

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$$

$$(\Delta A)_\psi = \sqrt{\langle \psi | \hat{A}^2 | \psi \rangle - \langle \psi | \hat{A} | \psi \rangle^2}$$

EXERCISE: Demonstrate that if $|\psi\rangle$ is an eigenket $|\varphi_m\rangle$ of an observable A, then we have a quantum state well-defined value of A characterized by:

① the probability of having as a result of measurement of A an eigenvalue a_n is:

$$P_n = \delta_{mn} = \begin{cases} 1 & \text{for } m = n \\ 0 & \text{for } m \neq n \end{cases}$$

② $\langle A \rangle_{\varphi_m} = a_m$

③ $\Delta A = 0$ (zero uncertainty)

SOLUTION: In this particular case of initial state given by an eigenstate φ_m of the operator $\hat{A}$, the random variable A of the measurement results become the deterministic quantity a_m (corresponding eigenvalue of $\hat{A}$)

that is the result of measurement of A is a_m with certainty (probability = 1)

① $P_n = F(\varphi_m, \varphi_n) = |\langle \varphi_m | \varphi_n \rangle|^2 = |\delta_{mn}|^2 = \delta_{mn}$

for orthonormalization of the eigenkets of the hermitian operator $\hat{A}$

② $\langle A \rangle_{\varphi_m} = \langle \varphi_m | \hat{A} | \varphi_m \rangle$

but $|\varphi_m\rangle$ is an eigenket: $\hat{A}|\varphi_m\rangle = a_m |\varphi_m\rangle$

$$\langle A \rangle_{\varphi_m} = \langle \varphi_m | a_m | \varphi_m \rangle$$

for the linearity of the scalar product in the 2nd term

$$= a_m \underbrace{\langle \varphi_m | \varphi_m \rangle}_{\text{normalized: } = 1} = a_m$$

③ $(\Delta A)^2_{\varphi_m} = \text{var}(A) = \langle (A - \langle A \rangle)^2 \rangle = \langle \varphi_m | (\hat{A} - \overbrace{\langle \varphi_m | \hat{A} | \varphi_m \rangle}^{= a_m})^2 | \varphi_m \rangle$

But:

$$(\Delta A)^2_{\varphi_m} = \langle \varphi_m | \underbrace{\hat{A}^2}_{a_m^2} | \varphi_m \rangle - \underbrace{\langle \varphi_m | \hat{A} | \varphi_m \rangle^2}_{a_m^2}$$

$$\hat{A}^2 |\varphi_m\rangle = \hat{A}(\hat{A}|\varphi_m\rangle) = \hat{A}(a_m |\varphi_m\rangle) = a_m \hat{A}|\varphi_m\rangle = a_m \cdot a_m |\varphi_m\rangle$$

$$= a_m^2 \, |\varphi_m\rangle$$

General property for observables A and B:

$$\begin{cases} \hat{B} = f(\hat{A}) \\ \hat{A}\,|\varphi_m\rangle = a_m\,|\varphi_m\rangle \end{cases} \Rightarrow \quad \hat{B}\,|\varphi_m\rangle = f(a_m)\,|\varphi_m\rangle$$

so we obtain:

$$(\Delta A)\,\varphi_m = \langle \varphi_m | a_m^2 | \varphi_m \rangle - a_m^2 = a_m^2 \underbrace{\langle \varphi_m | \varphi_m \rangle}_{=1} - a_m^2 = 0$$

EXPECTATION VALUE IN POSITION REPRESENTATION

Observable A with discrete spectrum (discrete set of eigenkets $|\varphi_n\rangle$ and eigenvalues a_n, with $n = 0, 1, 2, \ldots$)

The probability of measuring a_n is:

$$P_n = F(\psi, \varphi_n) = |\langle \varphi_n | \psi \rangle|^2 = \left| \iiint_{-\infty}^{+\infty} \varphi_n(x,y,z)\, \psi(x,y,z)\, dx\, dy\, dz \right|^2$$

(assuming normalized wave functions)

because in the position representation the quantum states are described by wave functions $\psi(x,y,z)$.

The expectation value becomes:

$$\langle A \rangle_\psi = \langle \psi | \hat{A} | \psi \rangle = \iiint_{-\infty}^{+\infty} \psi^*(x,y,z) \cdot \hat{A} \cdot \psi(x,y,z)\, dx\, dy\, dz$$

We consider now the case of continuous-spectrum position operator:

$$\hat{\vec{r}} = (\hat{x}, \hat{y}, \hat{z})$$

having expectation values of the cartesian components:

$$\langle x \rangle = \iiint_{-\infty}^{+\infty} \psi^*(x,y,z) \cdot \hat{x} \cdot \psi(x,y,z)\, dx\, dy\, dz$$

↳ $\hat{x}$ in position representation is just the multiplication by x

$$= \iiint_{-\infty}^{+\infty} \psi^*(x,y,z) \cdot x \cdot \psi(x,y,z)\, dx\, dy\, dz$$

$$= \iiint_{-\infty}^{+\infty} x \, |\psi(x,y,z)|^2\, dx\, dy\, dz$$

$P(x,y,z) \triangleq$ probability density function

$$\langle y \rangle = \iiint_{-\infty}^{+\infty} y \, |\psi(x,y,z)|^2\, dx\, dy\, dz$$

$$\langle z \rangle = \iiint_{-\infty}^{+\infty} z \, |\psi(x,y,z)|^2\, dx\, dy\, dz$$

$\langle x \rangle, \langle y \rangle, \langle z \rangle$ can be seen as the average coordinates of a 3-D continuous random variable with probability density function:

$$\rho(x,y,z) = |\Psi(x,y,z)|^2$$

> $\langle x \rangle, \langle y \rangle, \langle z \rangle$ can be also seen as the coordinates of the center of mass of a body with density (mass per unit volume)
>
> $$\rho(x,y,z) = |\Psi(x,y,z)|^2$$

In quantum mechanics:

$$\rho(x,y,z) = |\langle \varphi_{x,y,z} | \Psi \rangle|^2 \underset{\text{(Born's rule)}}{=} |\Psi(x,y,z)|^2$$

$\varphi_{x,y,z}$: position eigenstate having well-defined position value (x,y,z)

is the probability density function of the position of the particle:

$$\langle \varphi_{x,y,z} | \Psi \rangle = \iiint_{-\infty}^{+\infty} \varphi_{x,y,z}^*(\xi,\eta,\zeta) \cdot \Psi(\xi,\eta,\zeta)\, d\xi\, d\eta\, d\zeta$$

But the position eigenfunction is:

$$\varphi_{x,y,z}(\xi,\eta,\zeta) = \delta(\xi - x, \eta - y, \zeta - z)$$

$$\langle \varphi_{x,y,z} | \Psi \rangle = \iiint_{-\infty}^{+\infty} \delta^*(\xi - x, \eta - y, \zeta - z) \cdot \Psi(\xi,\eta,\zeta)\, d\xi\, d\eta\, d\zeta = \Psi(x,y,z)$$

EXPECTATION VALUE IN MOMENTUM REPRESENTATION

The quantum state is described by the "reciprocal-domain" (Fourier-domain) wave function:

$$\tilde{\Psi}(p_x, p_y, p_z) = \frac{1}{\sqrt{h^3}} \mathcal{F}\{\Psi(x,y,z)\}\Big|_{f_x = \frac{p_x}{h},\ f_y = \frac{p_y}{h},\ f_z = \frac{p_z}{h}}$$

$$= \frac{1}{\sqrt{h^3}} \iiint_{-\infty}^{+\infty} \Psi(x,y,z) \cdot e^{-2\pi i (f_x \cdot x + f_y \cdot y + f_z \cdot z)}\, dx\, dy\, dz$$

$$= \frac{1}{\sqrt{h^3}} \iiint_{-\infty}^{+\infty} \Psi(x,y,z) \cdot e^{-\frac{i}{h}(p_x \cdot x + p_y \cdot y + p_z \cdot z)}\, dx\, dy\, dz$$

$$= \frac{1}{\sqrt{h^3}} \iiint_{-\infty}^{+\infty} \Psi(\vec{r})\, e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\, d\vec{r}$$

The probability of measuring a_n for the observable A can be calculated as:

$$P_n = |\langle \varphi_n | \Psi \rangle|^2 = \left| \iiint_{-\infty}^{+\infty} \tilde{\varphi}_n(p_x, p_y, p_z) \cdot \tilde{\Psi}(p_x, p_y, p_z)\, dp_x\, dp_y\, dp_z \right|^2$$

The expectation value becomes:

$$\langle A \rangle_\varphi = \langle \Psi | \hat{A} | \Psi \rangle = \iiint_{-\infty}^{+\infty} \tilde{\Psi}^*(p_x, p_y, p_z) \cdot \hat{A}\, \tilde{\Psi}(p_x, p_y, p_z)\, dp_x\, dp_y\, dp_z$$

In the case of observable $\vec{p}$:

$$\langle p_x \rangle = \iiint_{-\infty}^{+\infty} \tilde{\Psi} \cdot \hat{p}_x\, \Psi\, dp_x\, dp_y\, dp_z = \iiint_{-\infty}^{+\infty} p_x \left| \tilde{\Psi}(p_x, p_y, p_z) \right|^2 dp_x\, dp_y\, dp_z$$

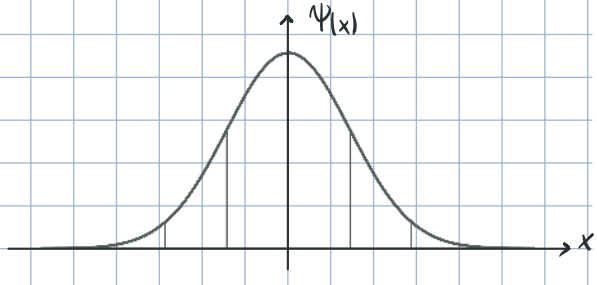
in the momentum representation is just a multiplication by p_x

EXERCISE: ① Calculate the condition so that a 1-D gaussian wave function is the fundamental (or ground) stationary state of the 1-D quantum harmonic oscillator.
(i.e. the minimum-energy eigenfunction Ψ_0 of $\hat{H}$)

② Calculate the expectation values and the uncertainties of position and momentum

SOLUTION: In position representation:

$$\Psi(x) = c \cdot e^{-ax^2}$$



$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$$

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

We want

$$\hat{H}\Psi_0(x) = E_0 \Psi_0(x)$$

(We can assume $c = 1$ for finding Ψ_0). We can calculate:

$$\frac{d^2}{dx^2} e^{-ax^2} = \frac{d}{dx}\left(\frac{d}{dx} e^{-ax^2}\right) = \frac{d}{dx}\left(-2ax\, e^{-ax^2}\right) = -2a \frac{d}{dx}\left(x\, e^{-ax^2}\right)$$

$$= -2a\left(1\cdot e^{-ax^2} + x\frac{d}{dx}e^{-ax^2}\right) = -2a\left[e^{-ax^2} + x\left(-2ax\right)\cdot e^{-ax^2}\right]$$

$$= \left(-2a + 4a^2x^2\right)e^{-ax^2}$$

$$\hat{H}\cdot e^{-ax^2} = \left[\frac{\hbar^2 a}{m} - \frac{2\hbar^2 a^2}{m}x^2 + \frac{1}{2}m\omega^2x^2\right]e^{-ax^2}$$

eigenvalue — must be cancelled to obtain a gaussian eigenfunction

$$\Downarrow$$

$$-\frac{2\hbar^2a^2}{m}x^2 + \frac{1}{2}m\omega^2x^2 = 0$$

hence:

$$a^2 = \frac{m}{2\hbar^2}\cdot\frac{m\omega^2}{2} = \frac{m^2\omega^2}{4\hbar^2} \longrightarrow a = \frac{m\omega}{2\hbar}$$

and we obtain the gaussian eigenfunction:

$$\psi_0(x) = c\cdot e^{-\frac{m\omega}{2\hbar}x^2}$$

Eigenvalue:

$$E_0 = \frac{\hbar^2 a}{m} = \frac{\hbar^2}{m}\cdot\frac{m\omega}{2\hbar} = \frac{1}{2}\hbar\omega \leftarrow \text{zero-point (ground) energy}$$

The Fourier transform of a gaussian function is still a gaussian function:

$$\mathcal{F}\left\{e^{-ax^2}\right\} = \sqrt{\frac{\pi}{a}}\,e^{-\frac{\pi^2 f_x^2}{a}}$$

EXERCISE: ① Calculate the condition so that a 1-D gaussian wave function is the fundamental (or ground) stationary state of the 1-D quantum harmonic oscillator.
(i.e. the minimum-energy eigenfunction ψ_0 of $\hat{H}$)

② Calculate the expectation values and the uncertainties of position and momentum

SOLUTION: [...]

We have found that the ground state $|\psi_0\rangle$ of the 1-D Q.H.O. is:

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

$$\hat{H}|\psi_0\rangle = E_0|\psi_0\rangle \qquad \text{with } E_0 = \frac{1}{2}\hbar\omega \quad \text{(zero-point energy)}$$

(In quantum physics, even at $T = 0K$, the particle has an uncertainty in both momentum and position, according to the Heisenberg's uncertainty principle. Even at absolute zero temperature the particle is not at rest).

We can then calculate $\langle x \rangle$ and Δx in the state $|\psi_0\rangle$. Expetation value of position:

$$\langle x \rangle_{\psi_0} = \langle \psi_0 | \hat{x} | \psi_0 \rangle = \int_{-\infty}^{+\infty} \psi_0^*(x) \cdot x \cdot \psi_0(x)\, dx =$$

(in position representation)

$$= \int_{-\infty}^{+\infty} x\, |\psi_0(x)|^2\, dx$$

$$= \int_{-\infty}^{+\infty} x\, \mathcal{P}_0(x)\, dx$$

$|\psi_0(x)|^2$: probability density function of measuring x.

$$\mathcal{P}_0(x) = |\psi_0(x)|^2 = |c|^2 \cdot e^{-\frac{m\omega}{\hbar}x^2}$$

⇓ it's a gaussian PDF

From the probability theory, the normalized gaussian is:

$$\mathcal{P}_0(x) = \frac{1}{\sqrt{2\pi}\cdot\sigma_x} \cdot e^{-\frac{x^2}{2\sigma_x^2}}$$

σ_x: standard deviation

$$\int_{-\infty}^{+\infty} |\psi_0(x)|^2\, dx = \int_{-\infty}^{+\infty} \mathcal{P}_0(x)\, dx = 1$$

We know that in this case the mean μ_x is zero and the standard deviation is σ_x:

$$\mu_x = 0$$

$$2\sigma_x^2 = \frac{\hbar}{m\omega} \longrightarrow \sigma_x = \sqrt{\frac{\hbar}{2m\omega}}$$

$$|c|^2 = \frac{1}{\sqrt{2\pi}\,\sigma_x} = \sqrt{\frac{m\omega}{\pi\hbar}} \longrightarrow c = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot \underbrace{e^{i\delta}}_{\text{generic phase term}}$$ with any possible δ (e.g. $\delta = 0$).

$$\Downarrow$$

$$\begin{cases} \langle x \rangle_{\psi_0} = \mu_x = 0 \\ (\Delta x)_{\psi_0} = \sigma_x = \sqrt{\frac{\hbar}{2m\omega}} \end{cases}$$

In fact, according to the definition, we have:

$$\langle x \rangle_{\psi_0} = \int_{-\infty}^{+\infty} \underbrace{x}_{\text{odd function of } x} \underbrace{\rho_x(x)}_{\text{even function of } x}\, dx = 0$$

the product is an odd function of x, so if we integrate an odd function over a symmetric interval we obtain 0

$$(\Delta x)_{\psi_0} = \langle (x - \cancel{\langle x \rangle})^2 \rangle_{\psi_0} = \langle x^2 \rangle_{\psi_0} - \cancel{\langle x \rangle_{\psi_0}^2}$$ ($\langle x \rangle = 0$, $\langle x \rangle^2 = 0$)

$$= \langle x^2 \rangle_{\psi_0} = \langle \psi_0 | \hat{x}^2 | \psi_0 \rangle$$

$$= \int_{-\infty}^{+\infty} \psi_0^*(x) \cdot x^2 \cdot \psi_0(x)\, dx = \int_{-\infty}^{+\infty} x^2 |\psi_0(x)|^2\, dx$$

$$= \int_{-\infty}^{+\infty} x^2 \rho_0(x)\, dx = \sigma_x^2$$

We calculate now $\langle p_x \rangle_{\psi_0}$ and $(\Delta p_x)_{\psi_0}$. In position representation:

$$\langle p_x \rangle_{\psi_0} = \langle \psi_0 | \hat{p}_x | \psi_0 \rangle = \int_{-\infty}^{+\infty} \underbrace{\psi_0^*(x)}_{\text{even}} \cdot \underbrace{(-i\hbar)\frac{d}{dx}}_{\text{odd}} \psi_0(x)\, dx = 0 \quad \text{(for symmetry)}$$

momentum operator in position representation

(We obtained, as for the expectation value of the position, the same result as can can be predicted by the classical vision of the (quantum) harmonic oscillator at the zero-energy point. What differenciate the two visions is the uncertainty on position and momentum of the particle).

$$(\Delta p_x)_{\psi_0}^2 = \langle (p_x - \cancel{\langle p_x \rangle})^2 \rangle_{\psi_0} = \langle p_x^2 \rangle_{\psi_0} = \langle \psi_0 | \hat{p}_x^2 | \psi_0 \rangle$$ ($\langle p_x \rangle = 0$)

$$= \int_{-\infty}^{+\infty} \psi_0^*(x) \cdot (-i\hbar)^2 \frac{d^2}{dx^2} \psi_0(x)\, dx = \dots$$

It is more convenient to use the momentum representation. "Reciprocal" wave function

(or canonically - conjugated wave function):

$$\tilde{\psi}_0(p_x) = \frac{1}{\sqrt{h}} F\{\psi_0(x)\}\Big|_{f_0 = \frac{p_x}{h}} = \frac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} \psi_0(x) \cdot e^{-i2\pi f_x x}\, dx \Big|_{f_x = \frac{p_x}{h}}$$

$$= \frac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} \psi_0(x) \cdot e^{-\frac{i}{\hbar} p_x \cdot x}\, dx$$

But the Fourier transform of a gaussian function is still a gaussian function with a reciprocal relation between the widths:

$$F\{e^{-ax^2}\} = \sqrt{\frac{\pi}{a}} \cdot e^{-\frac{\pi^2}{a} f_x^2} \qquad \text{with } a = \frac{m\omega}{2\hbar}$$

$$\tilde{\psi}_0(p_x) = D \cdot e^{-\pi^2 \left(\frac{p_x}{h}\right)^2 \cdot \frac{2\hbar}{m\omega}} = D \cdot e^{-\frac{p_x^2}{2\hbar m\omega}}$$

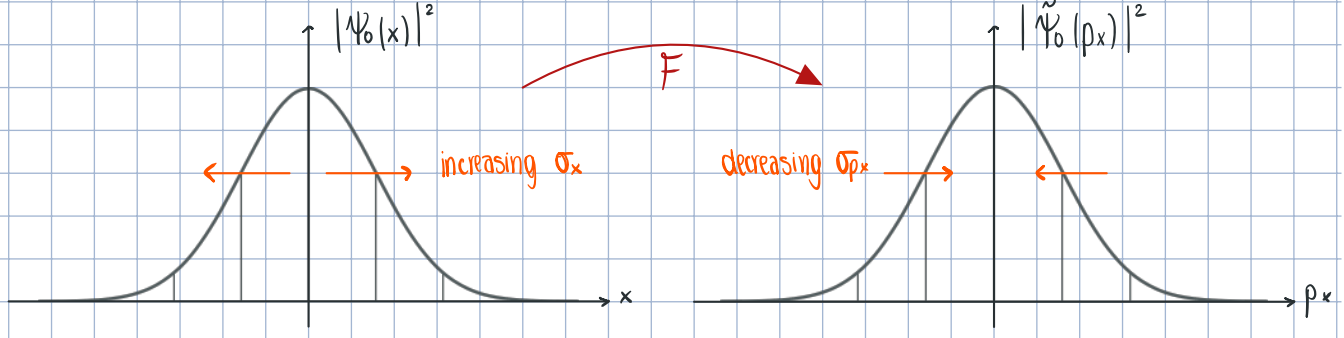
↓ multiplicative coefficient

The probability density function of measuring a value p_x for the momentum is:

$$\tilde{\rho}_0(p_x) = |\tilde{\psi}_0(p_x)|^2 = |D|^2 \cdot e^{-\frac{p_x^2}{\hbar m\omega}} \quad \frac{p_x^2}{\hbar m\omega} = 2\sigma_{p_x}^2$$

gaussian function with mean $\mu_{p_x} = 0$ and variance $\sigma_{p_x}^2 = \frac{\hbar m\omega}{2}$.

$$\begin{cases} \langle p_x \rangle_{\psi_0} = \mu_{p_x} = 0 \\ (\Delta p_x)_{\psi_0} = \sigma_{p_x} = \sqrt{\frac{\hbar m\omega}{2}} \end{cases}$$



$$(\Delta x)_{\psi_0} = \sqrt{\frac{\hbar}{2m\omega}}$$

$$(\Delta p_x)_{\psi_0} = \sqrt{\frac{\hbar m\omega}{2}}$$

$$\rightarrow \boxed{(\Delta x)_{\psi_0} (\Delta p_x)_{\psi_0} = \frac{\hbar}{2}}$$

For the Heisenberg's uncertainty principle this is the minimum possible value for the product

between uncertainties of position and momentum:

$$(\Delta x)_{\psi_0}(\Delta p_x)_{\psi_0} \geq \frac{\hbar}{2}$$

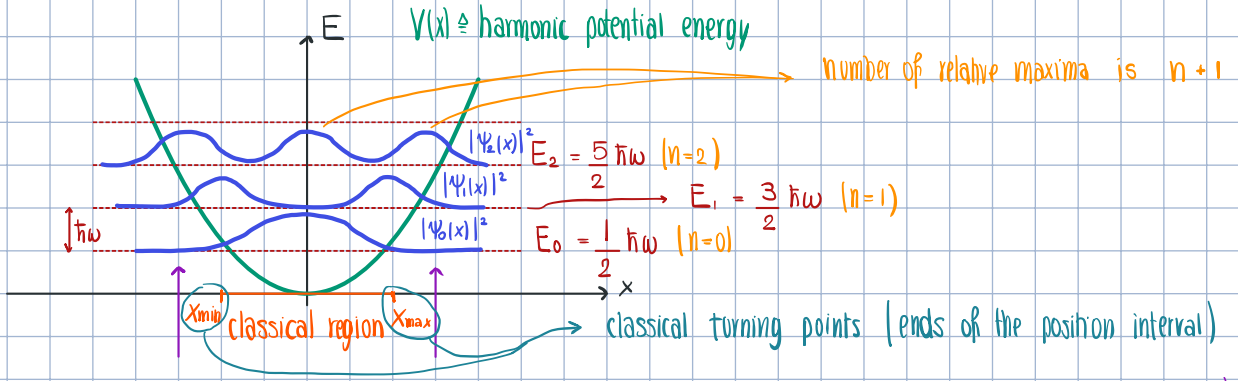
The gaussian wave function given by the ground-state eigenfunction of the Q.H.O. describes a "minimum uncertainty quantum state".

$|\psi_0\rangle$ is a "minimum uncertainty state".

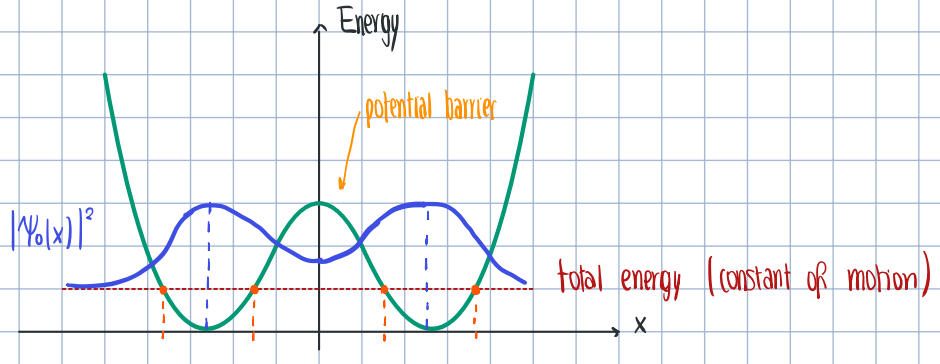
$|\psi_n\rangle$, with $n = 1, 2, 3, \ldots$, are NOT "minimum uncertainty state".

$\psi_n(x)$ are suitable hermite-gaussian function (for $n \neq 0$).

COHERENT STATES (of Q.H.O.)



quantum tunneling phenomenon (similar to the "evanescent wave" in classical physics)



classical turning points (kinetic energy = 0 => velocity = 0 => inversion of motion)

The coherent states are not-stationary states (not eigenstate of $\hat{H}$) for the Q.H.O. showing minimum product of uncertainties in position and momentum (minimum uncertainty states for the Q.H.O.).

$$|\alpha\rangle = \sum_{n=0}^{+\infty} e^{-\frac{|\alpha|^2}{2}} \cdot \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

NUMBER STATES → eigenkets of $\hat{H}$ $|\psi_n\rangle$ with eigenvalues $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$

With any complex number $\alpha = |\alpha| e^{i\delta}$

In position representation:

$$\psi_\alpha(x) = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{+\infty} \frac{\alpha^n}{\sqrt{n!}} \psi_n(x)$$

$\psi_n(x)$ → hermite-gaussian eigenfunctions of $\hat{H}$

The coherent state with $\alpha = 0$ is just the ground state

$$|0\rangle = |n = 0\rangle$$

$|0\rangle$: coherent state with $\alpha = 0$

$|n = 0\rangle$: $\psi_{\alpha=0}(x) = \psi_0(x)$ → ground-state eigenfunction

Consider an initial 1-D gaussian wave packet (a minimum-uncertainty wave function) with expectation values:

$\langle x \rangle = x_0$ at $t = 0$

$\langle p_x \rangle = p_0 = m v_0$ at $t = 0$

This wave packet can be seen as the quantum version of a classical body with initial position x_0 and initial velocity v_0 (in the quantum case we have uncertainties in position and momentum).

In general this gaussian wave packet is not a stationary state, so there will be an evolution of this state in time:

$$\Psi(x, t=0) = \psi(x) = c \cdot e^{-\frac{(x-x_0)^2}{4(\Delta x)_0^2}} \cdot e^{i K_x \cdot x}$$

($\vec{p} = \hbar \vec{K} \rightarrow K_x = \frac{p_x}{\hbar}$; $(\Delta x)_0$: uncertainty at time $t = 0$)

(Exercise: verify that $\langle p_x \rangle = \langle \psi | \hat{p}_x | \psi \rangle = p_0$)

We have $(\Delta x)_0 \cdot (\Delta p_x)_0 = \hbar/2$ for the Heisenberg's principle.

In the case of (1-D) Q.H.O., this gaussian wave packet evolves in time as a "coherent states" $|\alpha\rangle$ provided that $(\Delta x)_0 = \sqrt{\frac{\hbar}{2m\omega}}$

Moreover if $x_0 = 0$ and $p_0 = 0$ then the coherent state is the ground state $|\alpha\rangle = |0\rangle$

$$|\alpha\rangle = \sum_{n=0}^{+\infty} e^{-\frac{|\alpha|^2}{2}} \cdot \frac{\alpha^n}{\sqrt{n!}} |n\rangle \equiv |\psi_n\rangle$$

This state is not an eigenstate of $\hat{H}$ of the Q.H.O., but it is a superposition of eigenstates of $\hat{H}$ $\Rightarrow$ the coherent state is not a stationary state $\Rightarrow$ time evolution

$$\Psi(x,t) = \underbrace{e^{-\frac{i}{\hbar} t \hat{H}}}_{\text{time evolution operator}} \cdot \Psi(x,0) = e^{-\frac{i}{\hbar} t \hat{H}} \cdot \psi(x) = e^{-\frac{i}{\hbar} t \hat{H}} \cdot \sum_{n=0}^{+\infty} e^{-\frac{|\alpha|^2}{2}} \frac{\alpha^n}{\sqrt{n!}} \cdot \psi_n(x)$$

($\psi_n(x)$: eigenfunctions of $\hat{H}$ (hermite-gaussian functions))

$$= \underbrace{e^{-\frac{i}{\hbar} t \hat{H}}}_{\text{linear unitary operator}} \cdot \sum_n \lambda_n \psi_n(x)$$

$$= \sum_n \lambda_n \cdot e^{-\frac{i}{\hbar} t \hat{H}} \cdot \psi_n(x)$$

But $\psi_n(x)$ are eigenfunctions of $\hat{H}$ with eigenvalues:

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

and even eigenfunctions of $e^{-\frac{i}{\hbar}t\hat{H}}$ with eigenvalues $e^{-\frac{i}{\hbar}tE_n}$

$$e^{-\frac{i}{\hbar}t\hat{H}} \cdot \psi_n(x) = e^{-\frac{i}{\hbar}tE_n} \cdot \psi_n(x)$$

↳ complex number with modulus 1 (pure phase shift)

⇒ the time evolution of an eigenfunction of $\hat{H}$ is just a phase shift ⇒ the quantum state, in this case, does not change (STATIONARY STATE).

For the coherent state:

$$\Psi(x,t) = \sum_n \lambda_n \cdot e^{-i\frac{E_n}{\hbar}t} \cdot \psi_n(x)$$

It is possible to demonstrate that

$$|\Psi(x,t)|^2 = |c|^2 \cdot e^{-\frac{[x-\mu_x(t)]^2}{2(\Delta x)_0^2}}$$

with $\alpha = |\alpha| \cdot e^{i\delta}$

with $\langle x \rangle = \mu_x(t) = |\alpha| \cdot \sqrt{\frac{2\hbar}{m\omega}} \cdot \cos(\omega t - \delta)$

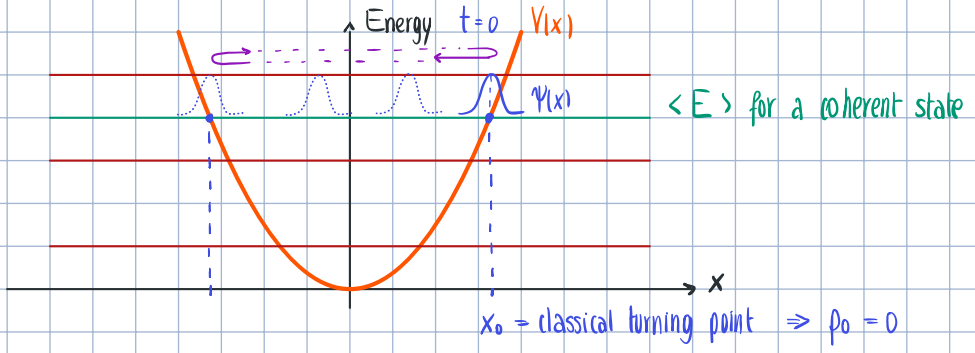
↳ harmonic oscillation of the center position of the wave packet following the same behaviour of the position of a body in the classical harmonic oscillator.

In general (for any quantum mechanical system):

$$\langle p_x \rangle = m \cdot \frac{d}{dt}\langle x \rangle$$

(extension to quantum mechanics of the classical definition: $p_x = m v_x = m\dot{x}$)

$$\langle p_x \rangle = -|\alpha|\sqrt{2m\omega\hbar} \cdot \sin(\omega t - \delta)$$



⟨E⟩ for a coherent state

this gaussian wave packet oscillates back and forth between the classical turning points with $\langle x \rangle$, $\langle p_x \rangle$ following the same rules of classical mechanics; the uncertainties Δx, Δp_x remain constant:

$$\begin{cases} \Delta x = \sqrt{\dfrac{\hbar}{2m\omega}} & \text{for any } t \geq 0 \\ \Delta p_x = \sqrt{\dfrac{\hbar m\omega}{2}} & \text{for any } t \geq 0 \end{cases}$$

$\longrightarrow$ NO spreading for the coherent states of the Q.H.O.

We consider now the (1-D) evolution of a gaussian wave packet in free-spaces (i.e. no forces on the particle $\Rightarrow$ $V(x) = 0$), with any initial uncertainty $(\Delta x)_0$.

We have:

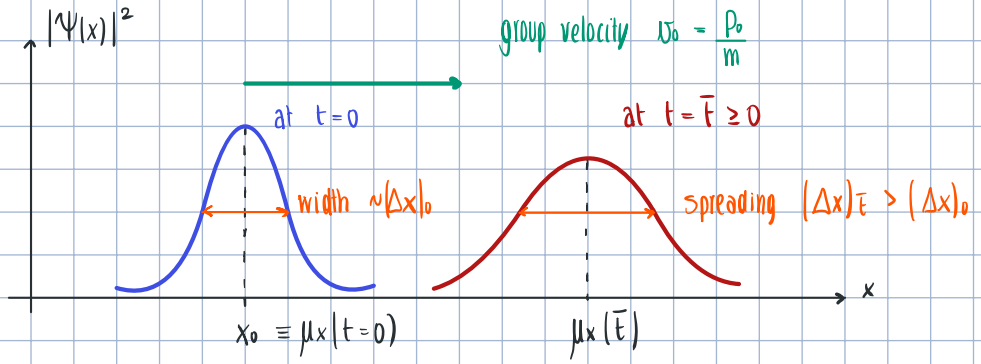
$$\langle p_x \rangle = m \langle v_x \rangle = m \cdot \frac{d}{dt} \langle x \rangle$$

with the initial conditions:

$$\begin{cases} \langle x \rangle = x_0 & \text{at } t = 0 \\ \langle p_x \rangle = p_0 & \text{at } t = 0 \end{cases}$$

and $\dfrac{d}{dt} \langle p_x \rangle = 0 \longrightarrow$ constant of motion (like in classical physics)

$\hookrightarrow$ $\langle p_x \rangle = p_0$ for any $t \geq 0$



$$\frac{d}{dt} \langle x \rangle = \frac{1}{m} \langle p_x \rangle = \frac{p_0}{m}$$

This is a general rule valid for any quantum mechanical system

$$\langle x \rangle = x_0 + \frac{p_0}{m} \cdot t \longrightarrow \mu_x(t) = x_0 + \frac{p_0}{m} \cdot t$$

The center of the wave packet moves at constant velocity (no forces $\Rightarrow$ inertial motion)

But there is the spreading of the wave packet (due to the Heisenberg's principle).

In classical mechanics, if there is a "spreading" $\Delta v_x = \Delta p_x / m$ of the velocity for a wave packet, then the "spreading" Δx after a time t is:

$$\Delta x = \Delta v_x \cdot t = \frac{\Delta p_x}{m} \cdot t$$

In quantum mechanics, we can consider the square of this Δx as an additional term expressing the increase of the variance (i.e. the square of the uncertainty) of the position for the wave packet:

$$\sigma_x^2(t) = (\Delta x)^2 = (\Delta x)_0^2 + \frac{(\Delta p_x)_0^2}{m^2} \cdot t^2$$

We are considering the initial uncertainty for momentum $(\Delta p_x)_0$, because for a free particle the momentum is a constant of motion in both classical and quantum mechanics.

A physical quantity is a "constant of motion" for a classical mechanical system if its value is constant (i.e. it does not change in the time).

Example: the energy of a mechanical system subject to a conservative (or non-dissipative) and time-independent field of forces (that is in case of existence of a time-independent potential energy) is a constant of motion.

Example: both momentum and angular momentum of a mechanical system not subject to any force (i.e. potential energy equal to zero) are constant of motion (inertial motion).

In quantum mechanics, an observable, is a "constant of motion" if the probability distribution of the random results of measurement does not change during time evolution of any initial quantum state. Hence, the expectation value and uncertainty of a constant of motion are time-independent for any quantum state.

Also in quantum physics, the momentum is a constant of motion for a free particle:

$$\begin{cases} \mu_{p_x} = \langle p_x \rangle = p_0 \\ \sigma_{p_x} = \Delta p_x = (\Delta p_x)_0 \end{cases}$$

for any time interval $0 \le t \le \bar{t}$ (in absence of quantum measurements in time interval)

Summarizing: ① Gaussian wave packet for quantum harmonic oscillator.

A gaussian wave packet with initial uncertainties:

$$\begin{cases} (\Delta x)_0 = \sqrt{\dfrac{\hbar}{2m\omega}} \\ (\Delta p_x)_0 = \sqrt{\dfrac{\hbar m\omega}{2}} \end{cases} \qquad \text{at } t = 0$$

remains a minimum-uncertainty wave packet, with constant uncertainties:

$$\begin{cases} \Delta x = \sqrt{\dfrac{\hbar}{2m\omega}} \\ \Delta p_x = \sqrt{\dfrac{\hbar m\omega}{2}} \end{cases} \qquad \text{for any } t \ge 0$$

$$\Rightarrow \boxed{(\Delta x)\cdot(\Delta p_x) = \frac{\hbar}{2}}$$

The corrisponding quantum state is a "coherent state", showing a time evolution of the expectation values of position and momentum according to the same laws of classical physics (that is harmonic motion).

② Free particle

The free particle is another example of quantum mechanical system showing a time evolution of expection values of position and momentum according to the usual classical rules (in this case giving an inertial motion, that is the momentum is constant of motion)

$$\begin{cases} \langle p_x \rangle = p_0 \\ \langle x \rangle = x_0 + \dfrac{p_0}{m} \cdot t \end{cases}$$

For any interval of time $0 \leq t \leq \bar{t}$ (in absence of measurements in the interval).

Being the momentum a constant of motion, the uncertainty of the momentum does not change in time

$$\Delta p_x = (\Delta p_x)_0 \qquad \text{for } 0 \leq t \leq \bar{t}$$

($\bar{t}$ can be seen as the instant of time of the first measurement after the initial preparation of the quantum state at $t = 0$).

In case of an initial minimum-uncertainty gaussian wave packet (at $t = 0$):

$$(\Delta x)_0 (\Delta p_x)_0 = \frac{\hbar}{2}$$

The wave packet remains gaussian in the time evolution, but with increasing uncertainty in position:

$$\Delta x = \sqrt{(\Delta x)_0^2 + \frac{(\Delta p_x)_0^2}{m^2} \cdot t^2} = \sqrt{(\Delta x)_0^2 + \frac{1}{(\Delta x)_0^2} \left(\frac{\hbar t}{2m}\right)^2}$$

and hence no more a minimum uncertainty wave packet for $t > 0$.

We have that x and p_x are canonically conjugated mechanical quantities (also in quantum mechanics):

$$[x] \cdot [p_x] = [\text{action}] \longrightarrow m \cdot \frac{kg \cdot m}{s} = kg \cdot \frac{m^2}{s} = J \cdot s$$

$$[t] \cdot [E] = [\text{action}] \longrightarrow s \cdot J = J \cdot s \quad \text{(equivalent)}$$

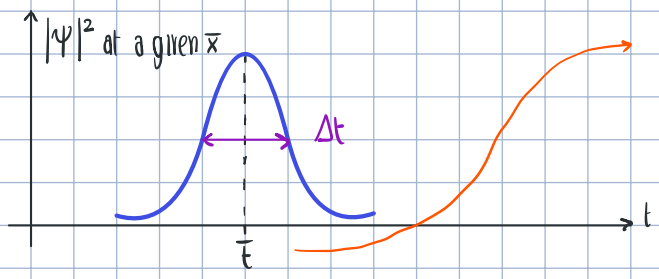
In quantum physics:

$$(\Delta x) \cdot (\Delta p_x) \geq \frac{\hbar}{2}$$

$$\boxed{(\Delta t) \cdot (\Delta E) \geq \frac{\hbar}{2}}$$

TIME-ENERGY UNCERTAINTY PRINCIPLE

It is not easy to demonstrate this principle because, in quantum mechanics, time is not an operator (observable), but we can intuitively derive this principle from the Heisenberg's uncertainty principle:



instant of time corresponding to the passage of the peak of the gaussian wave packet in $\bar{x}$.

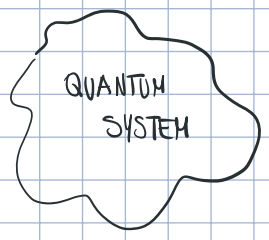
Wave packet of width Δx, moving at group velocity $v_0 = p_0/m$. But $v_0 = \Delta x/\Delta t$, so the uncertainty is

$$\Delta t = \frac{\Delta x}{v_0} = \frac{\Delta x_0}{p_0} \cdot m$$

and the energy uncertainty (in free space) is:

$$\Delta E = \Delta\left(\frac{p^2}{2m}\right) = \frac{d}{dp}\left(\frac{p^2}{2m}\right)\Big|_{p=p_0} \cdot \Delta p = \frac{p_0}{m} \cdot \Delta p$$

$$\Rightarrow \quad \Delta t \cdot \Delta E = \frac{\Delta x}{p_0} \cdot m \cdot \frac{p_0}{m} \cdot \Delta p = \Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$



Hilbert space $\mathcal{H}$ of kets to describe this system

It is possible to define a discrete orthonormal basis of $\mathcal{H}$:

$$\{ |\varphi_n\rangle \text{ , with } n = 0, 1, 2, \dots \}$$

For example we can consider the stationary states given by the eigenkets of $\hat{H}$, but we can choose the eigenkets of any observable.

We consider an operator $\hat{A}$ in $\mathcal{H}$, that is acting on kets:

$$|\psi'\rangle \xrightarrow{\hat{A}} |\psi''\rangle$$

"image", or "transformed vector" of $|\psi'\rangle$ by applying $\hat{A}$

$$|\psi''\rangle = \hat{A}\,|\psi'\rangle \qquad \text{(common formalism)}$$

LINEAR OPERATOR

It is characterized by the linearity property:

$$\hat{A}\left|\sum_n \lambda_n |\varphi_n\rangle\right\rangle = \sum_n \lambda_n \hat{A}\,|\varphi_n\rangle$$

All operators used in quantum mechanics are linear operators!

If we consider the expansion of any ket $|\psi\rangle$ in terms of the basis $\{|\varphi_n\rangle\}$, then

$$|\psi\rangle = \sum_n \lambda_n |\varphi_n\rangle$$

$$\hat{A}\,|\psi\rangle = \sum_n \lambda_n \hat{A}\,|\varphi_n\rangle$$

I have a complete knowledge of $\hat{A}$ when I know $\{\hat{A}\,|\varphi_n\rangle$, with $n = 0, 1, 2, \dots\}$

the set of kets which are the images of the basis kets

$$\hat{A}|\varphi_0\rangle \quad \hat{A}|\varphi_1\rangle \quad \dots \quad \hat{A}|\varphi_n\rangle \quad \dots$$

$$\begin{bmatrix} \langle\varphi_0|\hat{A}|\varphi_0\rangle \\ \langle\varphi_1|\hat{A}|\varphi_0\rangle \\ \vdots \\ \langle\varphi_m|\hat{A}|\varphi_0\rangle \\ \vdots \end{bmatrix} \quad \begin{bmatrix} \langle\varphi_0|\hat{A}|\varphi_1\rangle \\ \langle\varphi_1|\hat{A}|\varphi_1\rangle \\ \vdots \\ \langle\varphi_m|\hat{A}|\varphi_1\rangle \\ \vdots \end{bmatrix} \quad \dots \quad \begin{bmatrix} \langle\varphi_0|\hat{A}|\varphi_n\rangle \\ \langle\varphi_1|\hat{A}|\varphi_n\rangle \\ \vdots \\ \langle\varphi_m|\hat{A}|\varphi_n\rangle \\ \vdots \end{bmatrix} \quad \dots$$

n (column index), m (row index)

column 0 | column 1 | column n

If we merge all the columns:

$$\begin{bmatrix} & \vdots & \\ \cdots & A_{mn} = \langle \varphi_m | \hat{A} | \varphi_n \rangle & \cdots \\ & \vdots & \end{bmatrix}$$

the first index m is the raw-index

the second index n is the column-index

So we can say that:

linear operator $\hat{A}$ $\longleftrightarrow$ (representation on the chosen basis $\{|\varphi_n\rangle\}$) matrix with coefficients $A_{mn} = \langle \varphi_m | \hat{A} | \varphi_n \rangle$

For instance:

$|\psi''\rangle = \hat{A}\,|\psi'\rangle$ $\longleftrightarrow$ (representation)

$$\begin{bmatrix} \vdots \\ \lambda''_m = \langle \varphi_m | \psi'' \rangle \\ \vdots \end{bmatrix} = \underbrace{\begin{bmatrix} \vdots \\ \cdots A_{mn} = \langle \varphi_m | \hat{A} | \varphi_n \rangle \cdots \\ \vdots \end{bmatrix}}_{\text{matrix } D \times D} \cdot \underbrace{\begin{bmatrix} \vdots \\ \lambda'_n = \langle \varphi_n | \psi' \rangle \\ \vdots \end{bmatrix}}_{\text{column vector (matrix } D \times 1)}$$

usual matrix multiplication (raw by column multiplication):

$$\lambda''_m = \sum_{n=0}^{D-1} A_{mn}$$

(D is the dimension of $\mathcal{H}$)

Representation of the scalar product:

$\langle \psi' | \psi'' \rangle$ $\longleftrightarrow$ (representation)

$$\begin{bmatrix} \cdots & (\lambda'_n)^* & \cdots \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ \lambda''_n \\ \vdots \end{bmatrix} = \text{scalar (complex number)}$$

(matrix $1 \times D$) $\cdot$ (matrix $D \times 1$) = (matrix 1×1)

with $\begin{cases} (\lambda'_n)^* = \left(\langle \varphi_n | \psi' \rangle \right)^* = \langle \psi' | \varphi_n \rangle \\ \lambda''_n = \langle \varphi_n | \psi'' \rangle \end{cases}$

$$\Rightarrow \boxed{\langle \psi' | \psi'' \rangle = \sum_{n=0}^{D-1} (\lambda'_n)^* \cdot \lambda''_n}$$

Example: demonstrate the previous relation

$$\langle \psi' | \psi'' \rangle = \langle \psi' | \hat{1} \cdot \hat{1} | \psi'' \rangle \qquad \text{where } \hat{1} = \sum_{n=0}^{D-1} |\varphi_n\rangle\langle\varphi_n|$$

$$= \sum_m \langle \psi' | \varphi_m \rangle \langle \varphi_m | \sum_n |\varphi_n\rangle\langle\varphi_n|\psi''\rangle$$

$$= \sum_m (\lambda'_m)^* \langle \varphi_m | \sum_n \lambda''_n |\varphi_n\rangle$$

$$= \sum_m \sum_n (\lambda_m')^* \cdot \lambda_n'' \langle \varphi_m | \varphi_n \rangle \rightarrow \delta_{mn} \quad \text{(for the orthonormality of basis)}$$

$$= \sum_m \sum_n (\lambda_m')^* \cdot \lambda_n'' \, \delta_{mn}$$

$$= \sum_n (\lambda_n')^* \lambda_n''$$

The squared norm is:

$$\| \psi \|^2 = \langle \psi | \psi \rangle = \sum_n \lambda_n^* \cdot \lambda_n = \sum_n |\lambda_n|^2$$

DUAL OPERATOR

We start with a linear operator on the Hilbert space $\mathcal{H}$, that is an operator acting on Kets from left

$$|\psi''\rangle = \hat{A} |\psi'\rangle \xrightarrow{\text{duality transformation}} |\psi''\rangle^\dagger = (\hat{A} |\psi'\rangle)^\dagger = |\psi'\rangle^\dagger \hat{A}^\dagger$$

$$\langle \psi'' | = \langle \psi' | \hat{A}^{(\text{dual})}$$

$$\hat{A}^{(\text{dual})} \equiv \hat{A}^\dagger$$

The dual operator operates on the dual space $\mathcal{H}^*$, that acts on bras from right:

$$\langle \psi'' | = \langle \psi' | \hat{A}^\dagger \quad \xleftrightarrow{\text{representation in the orthonormal dual basis } \{\langle \varphi_n |, \text{ with } n = 0,1,2,\dots\}} \quad [\dots (\lambda_m'')^* \dots] = [\dots (\lambda_n')^* \dots] \cdot \begin{bmatrix} \vdots \\ \dots A_{nm}^\dagger \dots \\ \vdots \end{bmatrix}$$

(matrix $D \times 1$) (matrix $1 \times D$) (matrix $D \times D$)

$$(\lambda_m'')^* = \sum_{n=0}^{D-1} (\lambda_n')^* A_{nm}^\dagger \qquad \text{with} \quad \boxed{A_{nm}^\dagger = A_{mn}^*}$$

This means that the dual operator is represented $\hat{A}^\dagger$ is represented by a matrix which is the hermitian conjugate of the matrix representing $\hat{A}$.

The "$\dagger$" operation, in matrix operations, is the hermitian conjugation (or conjugate transposition)
(dagger)

EXERCISE: Demonstrate that

$$|\psi''\rangle = \hat{A}\,|\psi'\rangle \quad \xleftrightarrow{\text{representation}} \quad \begin{bmatrix} \vdots \\ \lambda_m'' \\ \vdots \end{bmatrix} = \begin{bmatrix} \cdots & \vdots & \cdots \\ & A_{mn} & \\ & \vdots & \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ \lambda_n' \\ \vdots \end{bmatrix}$$

with:

$$\lambda_m'' = \langle \varphi_m | \psi'' \rangle$$

$$\lambda_n' = \langle \varphi_n | \psi' \rangle$$

$$A_{mn} = \langle \varphi_m | \hat{A} | \varphi_n \rangle$$

SOLUTION: We have to demonstrate that

$$\lambda_m'' = \sum_n^{D-1} A_{mn} \cdot \lambda_n'$$

So we know that

expansion of the Ket to the superposition of the basis: $\sum_n |\varphi_n\rangle\langle\varphi_n|\psi'\rangle = \sum_n \lambda_n' |\varphi_n\rangle$

$$\lambda_m'' = \langle \varphi_m | \psi'' \rangle = \langle \varphi_m | \hat{A} | \psi' \rangle = \langle \varphi_m | \hat{A} \cdot \hat{1} | \psi' \rangle =$$

$$= \langle \varphi_m | \hat{A} \Big| \sum_n \lambda_n' | \varphi_n \rangle$$

for the linearity of the scalar product; for the linearity of $\hat{A}$

$$= \sum_n \lambda_n' \langle \varphi_m | \hat{A} | \varphi_n \rangle \quad \text{matrix coefficients } A_{mn}$$

$$= \sum_n \lambda_n' \cdot A_{mn} = \boxed{\sum_n^{D-1} A_{mn} \cdot \lambda_n'}$$

DUAL OPERATOR PROPERTIES

We have stated that if $\hat{A}$ is represented by $\begin{bmatrix} \cdots & \vdots & \cdots \\ & A_{mn} & \\ & \vdots & \end{bmatrix}$, then $\hat{A}^+ = \hat{A}^{(\text{dual})}$ is represented by:

$$\begin{bmatrix} \cdots & \vdots & \cdots \\ & A_{nm}^+ & \\ & \vdots & \end{bmatrix}$$

with $A_{nm}^+ = A_{mn}^*$.

The dagger ("+") operation on matrices is just the hermitian conjugation.

Demonstration: We know

the $\hat{A}$ operator acts from left on kets; duality operation "+"; the $\hat{A}^+$ operator acts from right on bras

$$|\psi\rangle = \hat{A}\,|\psi'\rangle \quad \xleftrightarrow{\text{duality operation "+"}} \quad \langle\psi| = \langle\psi'|\hat{A}^+$$

$$\Downarrow$$

$$\langle\psi''|\psi\rangle = \langle\psi''|\hat{A}|\psi'\rangle \quad \longleftrightarrow \quad \langle\psi|\psi''\rangle = \langle\psi'|\hat{A}^+|\psi''\rangle$$

For complex numbers (i.e. scalars): "$\dagger$" $\equiv$ "$*$". Indeed:

$$\langle \psi'' | \psi \rangle = \langle \psi | \psi'' \rangle^*$$

So we can equate the second sides of the two relation and then write:

$$\langle \psi' | \hat{A}^\dagger | \psi'' \rangle = \langle \psi'' | \hat{A} | \psi' \rangle^*$$

$$\underbrace{\langle \varphi_n | \hat{A}^\dagger | \varphi_m \rangle}_{A_{nm}^\dagger} = \underbrace{\langle \varphi_m | \hat{A} | \varphi_n \rangle^*}_{A_{mn}^*}$$

$$\boxed{A_{nm}^\dagger = A_{mn}^*} \quad \checkmark$$

ADJOINT OPERATOR

The symbol $\hat{A}^\dagger$ is used for both the dual operator $\hat{A}^{(dual)}$ and the adjoint operator $\hat{A}^{(adj)}$.

This ambiguity can be solved considering the action of the two operators in different Hilbert spaces.

$\hat{A}|\cdot\rangle$ is a linear operator in $\mathcal{H}$ (acting on kets from left)

$\langle \cdot | \hat{A}^{(dual)} = \langle \cdot | \hat{A}^\dagger$ is the dual operator in $\mathcal{H}^*$ (acting on bras from right)

$\hat{A}^{(adj)} | \cdot \rangle \equiv \hat{A}^\dagger | \cdot \rangle$ is the adjoint operator in $\mathcal{H}$ (acting on kets from left)

Both operators are represented by the same matrix:

$$\begin{bmatrix} \vdots \\ \cdots \; A_{mn}^\dagger \; \cdots \\ \vdots \end{bmatrix} \qquad \text{with} \quad A_{mn}^\dagger = A_{nm}^*$$

but acting in differents ways. We know that the representation of the action of $\hat{A}$ is the following matrix multiplication from left:

$$\begin{bmatrix} \vdots \\ \cdots \; A_{mn} \cdots \\ \vdots \end{bmatrix} \cdot \begin{bmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} = \begin{bmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

$$\begin{bmatrix} \cdot & \cdot & \cdot & \cdot \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ \cdots \; A_{mn}^\dagger \; \cdots \\ \vdots \end{bmatrix} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$A_{mn}^\dagger = A_{nm}^*$

The matrix $A^\dagger$ representing the dual operator multiplies the bra from right.

$$\begin{bmatrix} \cdots & \vdots \\ & A^{\dagger}_{mn} \\ & \vdots \end{bmatrix} \cdot \begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix} = \begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

$A^{\dagger}_{mn} = A^{*}_{nm}$

The matrix $A^{\dagger}$ representing the adjoint operator multiplies the ket from left.

Example:

$$\langle \psi' | \hat{A}^{\dagger} | \psi'' \rangle = \begin{cases} \textcircled{1}\ \left(\langle \psi' | \hat{A}^{(\text{dual})}\right) | \psi'' \rangle \\ \langle \psi' | \left(\hat{A}^{(\text{adj})} | \psi'' \rangle\right) \ \textcircled{2} \end{cases}$$

} two interpretations

representation

$$\textcircled{1}\ \left(\begin{bmatrix} \cdots & (\lambda'_m)^* & \cdots \end{bmatrix} \left(\cdot \begin{bmatrix} \cdots & \vdots \\ & A^{\dagger}_{mn} \\ & \vdots \end{bmatrix} \right) \cdot \begin{bmatrix} \vdots \\ \lambda''_n \\ \vdots \end{bmatrix} \right) \textcircled{2}$$

The matrix product is associative ⟶ no ambiguity !

The dagger operation ("†") is anti-distributive:

$$(A \cdot B)^{\dagger} = B^{\dagger} \cdot A^{\dagger}$$

This fundamental property can be demonstrated by using the matrix representation (and then is valid in general). The dagger "†" in matrix algebra is the "hermitian conjugation" (conjugate transposition).

Another property of dagger "†" is

$$(A^{\dagger})^{\dagger} = A \qquad (\text{"}\dagger^{-1}\text{"} \equiv \text{"}\dagger\text{"})$$

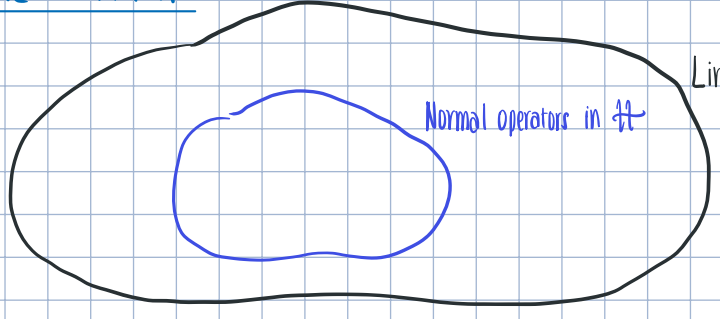
EXERCISE:

$$\langle \psi' | \hat{A}^{\dagger} | \psi'' \rangle = \left(\langle \psi' | \hat{A}^{\dagger} | \psi'' \rangle^{\dagger} \right)^{\dagger} = \left(| \psi'' \rangle^{\dagger} (\hat{A}^{\dagger})^{\dagger} \langle \psi' |^{\dagger} \right)^{\dagger} =$$

$$= \langle \psi'' | \hat{A} | \psi' \rangle^{\dagger}$$

$$= \langle \psi'' | \hat{A} | \psi' \rangle^{*}$$

NORMAL OPERATORS



$\hat{A}$ is a <u>normal operator</u> when $\hat{A}$ is a linear operator commuting with its adjoint:

$$\hat{A}\cdot\hat{A}^{\dagger} = \hat{A}^{\dagger}\cdot\hat{A}$$

We consider two linear operators $\hat{A}, \hat{B}$ in $\mathcal{H}$:

$$\hat{A}\cdot\hat{B}\,|\psi\rangle = \hat{A}\cdot\left(\hat{B}\,|\psi\rangle\right)$$

$$\hat{B}\cdot\hat{A}\,|\psi\rangle = \hat{B}\cdot\left(\hat{A}\,|\psi\rangle\right)$$

The linear operator $\hat{A}\cdot\hat{B}$ is represented by the matrix product:

$$\begin{bmatrix} \vdots \\ \cdots\ A_{mn}\ \cdots \\ \vdots \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ \cdots\ B_{mn}\ \cdots \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \cdots\ C_{mn}\ \cdots \\ \vdots \end{bmatrix}$$

The product between operators (matrices) is not commutative, so in general

$$\hat{A}\cdot\hat{B} \neq \hat{B}\cdot\hat{A}$$

If $\hat{A}\cdot\hat{B} = \hat{B}\cdot\hat{A}$, then $\hat{A}, \hat{B}$ are commuting operators (i.e. they commute).

Fundamental theorems for normal operators

$\hat{A}$ is a normal operator in $\mathcal{H}$ $\Longleftrightarrow$ (※) it exists an orthonormal basis of $\mathcal{H}$ formed by eigenvectors of $\hat{A}$

$\Downarrow$ $\uparrow$ (★)

$\hat{A}$ has a spetral decomposition in an orthonormal basis:

$$\hat{A} = \sum_{n=0}^{D-1} a_n \hat{\Pi}_n \underset{(*)}{=} \sum_n a_n |\varphi_n\rangle\langle\varphi_n|$$

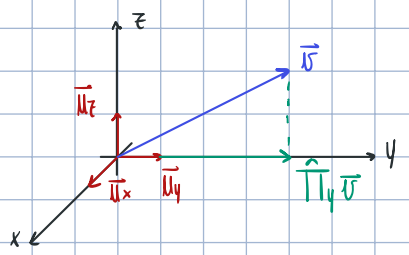
$\hat{\Pi}_n = |\varphi_n\rangle\langle\varphi_n|$ is an orthogonal projector on the normalized Ket $|\varphi_n\rangle$

(if this condition (*) is verified then a_n are the eigenvalues of $\hat{A}$ and $|\varphi_n\rangle$ are the corrisponding eigenKets).

The "spectrum" of an operator is the set of its eigenvalues.

Demonstration of (☆) : We introduced the property of the orthonogonal projector on $|\varphi\rangle$

$$\hat{\Pi}_n = |\varphi_n\rangle\langle\varphi_n|$$



$$\begin{cases} \hat{\Pi}_y \vec{u}_y = \vec{u}_y \rightarrow \text{eigenvector with eigenvalue 1} \\ \hat{\Pi}_y \vec{u}_z = 0 = 0 \cdot \vec{u}_z \rightarrow \text{" " " " 0} \\ \hat{\Pi}_y \vec{u}_x = 0 = 0 \cdot \vec{u}_x \rightarrow \text{" " " " 0} \end{cases}$$

$$\hat{\Pi}_n |\varphi_m\rangle = |\varphi_n\rangle \overbrace{\langle\varphi_n|\varphi_m\rangle}^{\delta_{nm}} = |\varphi_n\rangle \delta_{nm} = \begin{cases} |\varphi_m\rangle & \text{when } n = m \\ 0 & \text{when } n \neq m \end{cases}$$

Hyp.: $\hat{A} = \sum_{n=0}^{D-1} a_n \hat{\Pi}_n = \sum_n a_n |\varphi_n\rangle\langle\varphi_n|$

with $\{|\varphi_n\rangle\}$ an orthonormal basis.

$$\hat{A}|\varphi_m\rangle = \sum_n a_n |\varphi_n\rangle\langle\varphi_n|\varphi_m\rangle = \sum_n a_n |\varphi_n\rangle \delta_{nm} = a_m |\varphi_m\rangle$$

So we have demonstrated that a_m is eigenvalue of $\hat{A}$ with eigenkets $|\varphi_m\rangle$.

$\Rightarrow$ $\hat{A}$ admits an orthonormal basis formed by eigenkets $\{|\varphi_m\rangle\}$ ✓

Demonstration of (※) : Hyp: $\hat{A} = \sum_n a_n |\varphi_n\rangle\langle\varphi_n|$

We can see that if $\hat{A}$ is normal, then also $\hat{A}^+$ is normal with same eigenkets and complex conjugated eigenvalues :

$$\hat{A}^+ = \left(\sum_m a_m |\varphi_m\rangle\langle\varphi_m|\right)^+$$

↓ for linearity of the dagger operation

$$= \sum_m \left(a_m |\varphi_m\rangle\langle\varphi_m|\right)^+$$

↓ for anti-distributive property of dagger

$$= \sum_m \langle\varphi_m|^+ \cdot |\varphi_m\rangle^+ \cdot a_m^+$$

$$= \sum_m |\varphi_m\rangle\langle\varphi_m| \cdot a_m^*$$

$$= \sum_m a_m^* |\varphi_m\rangle\langle\varphi_m|$$

$$= \sum_m a_m^* \Pi_m \qquad (\text{indeed } \Pi_m^+ = \Pi_m)$$

Now we can calculate the product :

$$\hat{A}\cdot\hat{A}^\dagger = \sum_n a_n |\varphi_n\rangle\langle\varphi_n| \cdot \sum_m a_m^* |\varphi_m\rangle\langle\varphi_m|$$

$$= \sum_n a_n |\varphi_n\rangle \sum_m a_m^* \underbrace{\langle\varphi_n|\varphi_m\rangle}_{\delta_{nm}} \langle\varphi_m|$$

$$= \sum_n \sum_m a_n a_m^* |\varphi_n\rangle \delta_{nm} \langle\varphi_m|$$

$$= \sum_n a_n \cdot a_n^* |\varphi_n\rangle\langle\varphi_n|$$

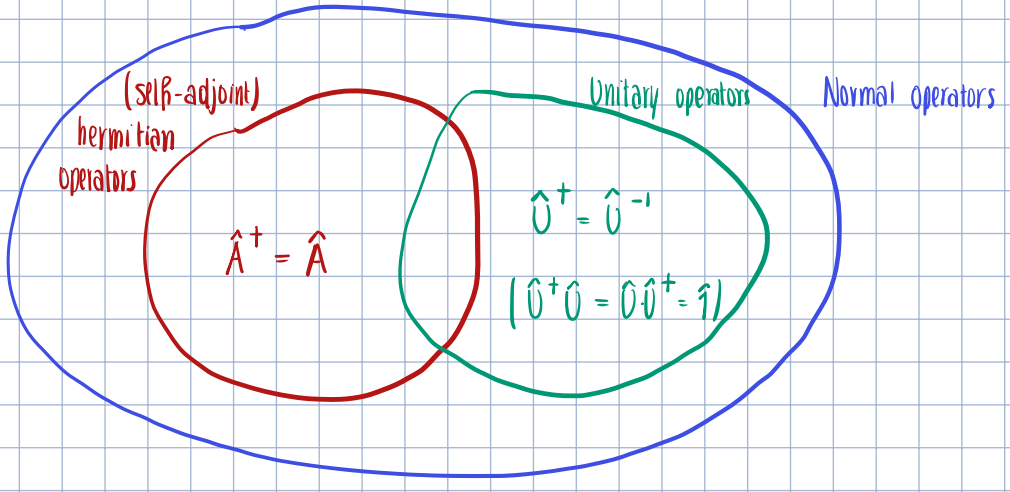
$$= \sum_n |a_n|^2 \cdot \hat{\Pi}_n$$

So the operator $\hat{A}\cdot\hat{A}^\dagger$ is a normal operator with eigenkets $|\varphi_n\rangle$ and eigenvalues $|a_n|^2$.

But also

$$\hat{A}^\dagger\cdot\hat{A} = \sum_n a_n^* \cdot a_n \cdot \hat{\Pi}_n = \sum_n |a_n|^2 \cdot \hat{\Pi}_n$$

and hence $\hat{A}\cdot\hat{A}^\dagger = \hat{A}^\dagger\cdot\hat{A}$ ✓



We want to represent a normal operator in terms of matrix representation:

$$\hat{A}\cdot\hat{A}^\dagger = \hat{A}^\dagger\cdot\hat{A}$$

matrix representation ⟷ in a given orthonormal basis

normal matrix:

$$\begin{bmatrix} \vdots \\ \cdots A_{mn} \cdots \\ \vdots \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ \cdots A_{nm}^* \cdots \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \cdots A_{nm}^* \cdots \\ \vdots \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ \cdots A_{mn} \cdots \\ \vdots \end{bmatrix}$$

A normal operator $\hat{A}$ is represented by a diagonal matrix in the orthonormal basis formed by its eigenvectors:

$$\begin{bmatrix} \vdots \\ \cdots A_{mn} \cdots \\ \vdots \end{bmatrix} = \begin{bmatrix} a_0 & 0 & \cdots & 0 \\ 0 & a_1 & 0 & \vdots \\ 0 & 0 & \ddots & \\ \vdots & \vdots & & a_n \; 0 \\ 0 & 0 & \cdots & \ddots \end{bmatrix}$$

with $a_0, a_1, a_2, \ldots$ given by the eigenvalues of $\hat{A}$

The matrix coefficients of a diagonal matrix are:

$$A_{mn} = a_n \delta_{mn} = \begin{cases} a_n & \text{for } m = n \\ 0 & \text{for } m \neq n \end{cases}$$ (diagonal elements)

$$A_{mn} = \langle \varphi_m | \hat{A} | \varphi_n \rangle$$ where $\{ |\varphi_n\rangle, n = 0,1,2,\ldots \}$ is the orthonormal basis formed by eigenkets

$$\hat{A}|\varphi_n\rangle = a_n |\varphi_n\rangle$$

$$\Downarrow$$

$$A_{mn} = \langle \varphi_m | a_n | \varphi_n \rangle = a_n \langle \varphi_m | \varphi_n \rangle = a_n \cdot \delta_{mn}$$

(for the linearity of the scalar product)

COMMUTATION OPERATOR

In general

$$\hat{A}\cdot\hat{B} \neq \hat{B}\cdot\hat{A}$$

It is useful to define the commutating operator (or "commutator"):

$$[\hat{A}, \hat{B}] = \hat{A}\cdot\hat{B} - \hat{B}\cdot\hat{A}$$

Two linear operators $\hat{A}, \hat{B}$ commute if and only if $[\hat{A}, \hat{B}] = 0$

Theorem: two normal operators $\hat{A}, \hat{B}$ are commuting operators (i.e. $[\hat{A}, \hat{B}] = 0$) if and only if $\hat{A}, \hat{B}$ are linear operators and it exists an orthonormal basis formed by a set of common eigenkets $\{|\varphi_n\rangle,\ n = 0, 1, 2, \dots\}$:

(common eigenkets = eigenkets of both operators)

$$\begin{cases} \hat{A}\,|\varphi_n\rangle = a_n\,|\varphi_n\rangle \\ \hat{B}\,|\varphi_n\rangle = b_n\,|\varphi_n\rangle \end{cases}$$

(☆)

Demonstration of (☆): Hyp.: $\hat{A}, \hat{B}$ are normal with the same eigenkets.

$$\hat{A} = \sum_n a_n \hat{\Pi}_n = \sum_n a_n\,|\varphi_n\rangle\langle\varphi_n|$$

$$\hat{B} = \sum_m b_m \hat{\Pi}_m = \sum_m b_m\,|\varphi_m\rangle\langle\varphi_m|$$

$$\hat{A}\cdot\hat{B} = \left(\sum_n a_n\,|\varphi_n\rangle\langle\varphi_n|\right)\left(\sum_m b_m\,|\varphi_m\rangle\langle\varphi_m|\right)$$

$$= \sum_n \sum_m a_n b_m\,|\varphi_n\rangle\underbrace{\langle\varphi_n|\varphi_m\rangle}_{\delta_{nm}}\langle\varphi_m|$$

$$= \sum_n \sum_m a_n b_m \delta_{nm}\,|\varphi_n\rangle\langle\varphi_m|$$

$$= \sum_n a_n b_n\,|\varphi_n\rangle\langle\varphi_m| = \sum_n a_n b_n \cdot \hat{\Pi}_n$$

We obtained that $\hat{A}\cdot\hat{B}$ is another normal operator with same eigenkets $\{|\varphi_n\rangle\}$ of $\hat{A}$ and $\hat{B}$ and with eigenvalues $a_n \cdot b_n$

$$\hat{B}\cdot\hat{A} = \dots = \sum_n b_n a_n\,|\varphi_n\rangle\langle\varphi_n| = \sum_n b_n a_n \hat{\Pi}_n = \hat{A}\cdot\hat{B}$$

We have demonstrated that

$$[\hat{A}, \hat{B}] = \hat{A}\cdot\hat{B} - \hat{B}\cdot\hat{A} = 0 \quad \checkmark$$

In this case, choosing as basis $\{|\varphi_n\rangle\}$ the diagonal matrix representation is:

$$A\cdot B = B\cdot A = \begin{bmatrix} a_0 b_0 & & & \\ & a_1 b_1 & & 0 \\ & & \ddots & \\ & 0 & & a_n b_n \\ & & & & \ddots \end{bmatrix}$$

HERMITIAN OPERATORS (or self-adjoint operators)

Definition of hermitian operator:

$$\hat{A}^\dagger = \hat{A}$$

(88)

An hermitian operator can be seen as a (normal) operator $\hat{A}$ having a spectral decomposition with all real eigenvalues.

Example: demonstrate that an hermitian operator is also normal.

Hyp.: $\hat{A}^\dagger = \hat{A}$

So we can write:

$$\hat{A}\cdot\hat{A}^\dagger = \hat{A}\cdot\hat{A} = \hat{A}^2$$

$$\hat{A}^\dagger\cdot\hat{A} = \hat{A}\cdot\hat{A} = \hat{A}^2$$

Hence:

$$\hat{A}\cdot\hat{A}^\dagger = \hat{A}^\dagger\cdot\hat{A}$$

Demonstration of (88): Hyp: $\hat{A} = \sum_n a_n |\varphi_n\rangle\langle\varphi_n|$ (a_n: real eigenvalues $(a_n^* = a_n)$; $|\varphi_n\rangle$: eigenkets)

$$\hat{A}^\dagger = \left(\sum_n a_n |\varphi_n\rangle\langle\varphi_n|\right)^\dagger = \left(\sum_n a_n \hat{\Pi}_n\right)^\dagger = \sum_n a_n^* \hat{\Pi}_n^\dagger$$

$$= \sum_n a_n \hat{\Pi}_n \quad \checkmark$$

the orthogonal projectors are hermitian operators

$$\hat{\Pi}_n = |\varphi_n\rangle\langle\varphi_n|$$

$$\hat{\Pi}_n^\dagger = \left(|\varphi_n\rangle\langle\varphi_n|\right)^\dagger = \langle\varphi_n|^\dagger |\varphi_n\rangle^\dagger = |\varphi_n\rangle\langle\varphi_n|$$

Demonstration that all eigenvalues of an hermitian operator are real:

Hyp: $\hat{A}^\dagger = \hat{A}$

$$\hat{A}|\varphi_n\rangle = a_n|\varphi_n\rangle$$

$\langle\varphi_n|\hat{A}|\varphi_n\rangle$ = expectation value of $\hat{A}$ in the eigenket $|\varphi_n\rangle$ must be equal to the eigenvalue a_n

$$= a_n \underbrace{\langle\varphi_n|\varphi_n\rangle}_{=1} = a_n$$

We now have to consider the dual expression:

$$\left(\hat{A}\,|\varphi_n\rangle\right)^{\dagger} = \left(a_n\,|\varphi_n\rangle\right)^{\dagger}$$

$$\langle\varphi_n|\hat{A}^{\dagger} = \langle\varphi_n|a_n^{*} = a_n^{*}\langle\varphi_n|$$

$$\langle\varphi_n|\hat{A}^{\dagger}|\varphi_n\rangle = a_n^{*}\langle\varphi_n|\varphi_n\rangle = a_n^{*}$$

But we have obtained:

$$\langle\varphi_n|\hat{A}|\varphi_n\rangle = a_n$$

By hypothesis, $\hat{A}^{\dagger} = \hat{A} \Rightarrow a_n = a_n^{*}$

So each eigenvalue a_n is real. ✓

Demonstrate: If $a' \neq a''$ are two differents eigenvalues of an hermitian operator, then the corrisponding eigenstates are orthogonal.

Hyp.: $\left.\begin{aligned}\hat{A}\,|\psi'\rangle &= a'\,|\psi'\rangle\\ \hat{A}\,|\psi''\rangle &= a''\,|\psi''\rangle\end{aligned}\right\}$ with $a' \neq a''$

It is convenient for evidencing the scalar product to close the first expression with $\langle\psi''|$ and the second with $\langle\psi'|$:

① $\begin{cases}\langle\psi''|\hat{A}|\psi'\rangle = a'\langle\psi''|\psi'\rangle\\ \langle\psi'|\hat{A}|\psi''\rangle = a''\langle\psi'|\psi''\rangle\end{cases}$ "$*$" or "$\dagger$"

② $\langle\psi'|\hat{A}|\psi''\rangle^{\dagger} = \left(a''\langle\psi'|\psi''\rangle\right)^{\dagger}$

$\langle\psi''|\hat{A}^{\dagger}|\psi'\rangle = \underbrace{(a'')^{*}}_{=a''}\langle\psi''|\psi'\rangle$

But we know the operator is hermitian ($\hat{A}^{\dagger} = \hat{A}$), hence:

$$\langle\psi''|\hat{A}^{\dagger}|\psi'\rangle = \langle\psi''|\hat{A}|\psi'\rangle$$

So we can write:

① $\langle\psi''|\hat{A}|\psi'\rangle = a'\langle\psi''|\psi'\rangle$

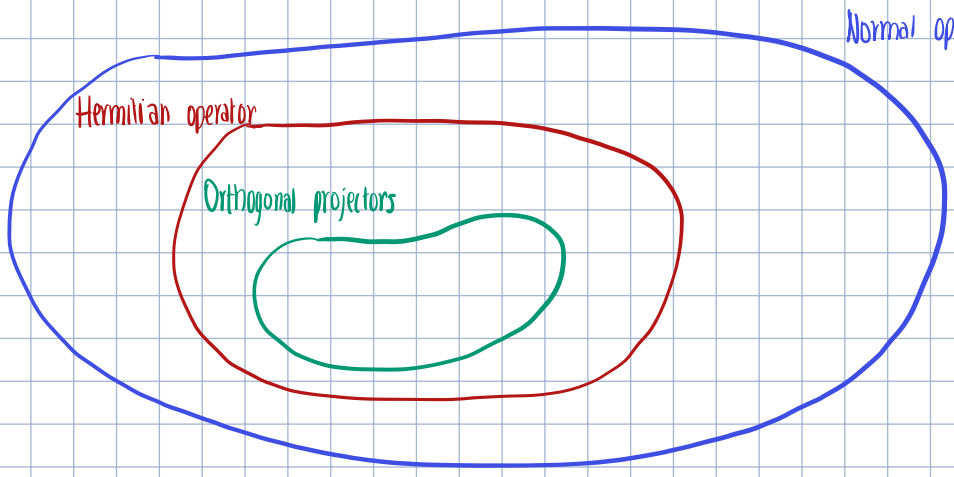
② $\langle\psi''|\hat{A}^{\dagger}|\psi'\rangle = a''\langle\psi''|\psi'\rangle$

$\Rightarrow \quad (a''-a')\langle\psi''|\psi'\rangle = 0$

But $a' \neq a''$ by hypothesis $\Rightarrow$ $\langle \psi'' | \psi' \rangle = 0$

So we have demonstrate that the eigenkets $|\psi'\rangle$, $|\psi''\rangle$ are orthogonal. ✓

ORTHOGONAL PROJECTOR

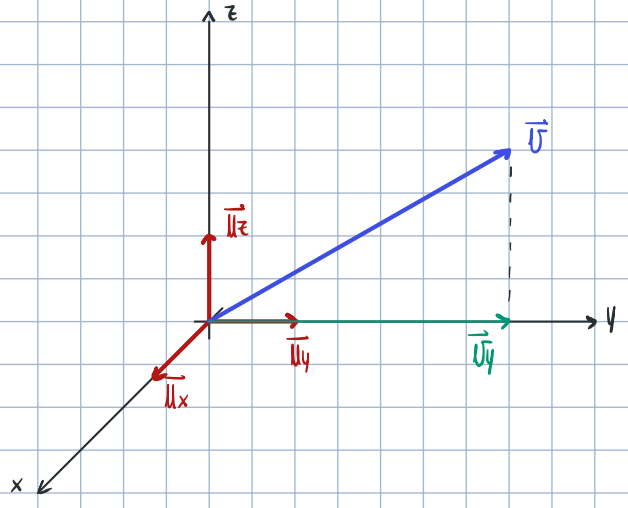


An orthogonal projector $\hat{\Pi}$, by definition, is an hermitian operator $(\hat{\Pi}^+ = \hat{\Pi})$, with the property $\hat{\Pi}^2 = \hat{\Pi}$ IDEMPOTENCE PROPERTY: $\hat{\Pi}^n = \hat{\Pi}$ (for any integer $n \geq 1$)

Example: $\hat{\Pi}^3 = \hat{\Pi} \cdot \hat{\Pi}^2 = \hat{\Pi} \cdot \hat{\Pi} = \hat{\Pi}^2 = \hat{\Pi}$

$\hat{\Pi}^n = \hat{\Pi} \cdot \hat{\Pi}^{n-1} = \dots = \hat{\Pi}$

Orthogonal projectors in euclidian geometry:



Versors $\vec{u}_x, \vec{u}_y, \vec{u}_z$ (length equal to 1)

$\vec{v} = \vec{v}_x + \vec{v}_y + \vec{v}_z = v_x \cdot \vec{u}_x + v_y \cdot \vec{u}_y + v_z \cdot \vec{u}_z$

Scalar components: $\begin{cases} v_x = \vec{u}_x \cdot \vec{v} \\ v_y = \vec{u}_y \cdot \vec{v} \\ v_z = \vec{u}_z \cdot \vec{v} \end{cases}$

The vector projection of $\vec{v}$ along z axis is:

$\vec{v}_y = v_y \cdot \vec{u}_y = (\vec{u}_y \cdot \vec{v}) \cdot \vec{u}_y$

scalar coefficient of the projection along y-axis

$$\Pi_y \cdot \vec{v} = \vec{v}_y = (\vec{u}_y \cdot \vec{v})\,\vec{u}_y$$

Obviously we have that :

$$\Pi_y^2 \vec{v} = \vec{v}_y = \Pi_y \vec{v}_y$$

hence :

$$\Pi_y^2 = \Pi_y$$

$\Rightarrow$ idempotence of orthonormal projector in euclidian geometry.

So we have :

$$\Pi_y \cdot \vec{v} = (\vec{u}_y \cdot \vec{v})\cdot \vec{u}_y \xrightarrow[\text{Hilbert spaces}]{\text{generalization to}} \hat{\Pi}_m |\psi\rangle = \underbrace{\left(\langle \varphi_m | \psi \rangle\right)}_{\text{scalar coefficient in the expansion of } \psi = \lambda_m} |\varphi_m\rangle$$

$$= |\varphi_m\rangle \lambda_m \quad \text{for any ket } |\psi\rangle$$

$$\downarrow$$

$$\boxed{\hat{\Pi}_m = |\varphi_m\rangle\langle\varphi_m|}$$

ORTHOGONAL PROJECTOR

↳ Hilbert space $\mathcal{H}$ dimension (finite or infinite)

An orthogonal projector of rank r ($0 \leq r \leq D$, with r integer) is defined as the orthogonal projector (i.e. an idempotent hermitian operator) in a subspace Σ_r of dimension r of the Hilbert space $\mathcal{H}$ that can be written as:

$$\hat{\Pi}_{\Sigma_r} = \sum_{n=1}^{r} |\varphi_n\rangle\langle\varphi_n|$$

where $\{|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_r\rangle\}$ is the orthonormal basis of the subspace Σ_r.

In general, the rank of a linear operator is the dimension of the subspace formed by all the image vector.

In case of rank $r = 1$ we obtain the orthogonal projector in a single quantum space:

$$\hat{\Pi}_\varphi = |\varphi\rangle\langle\varphi|$$

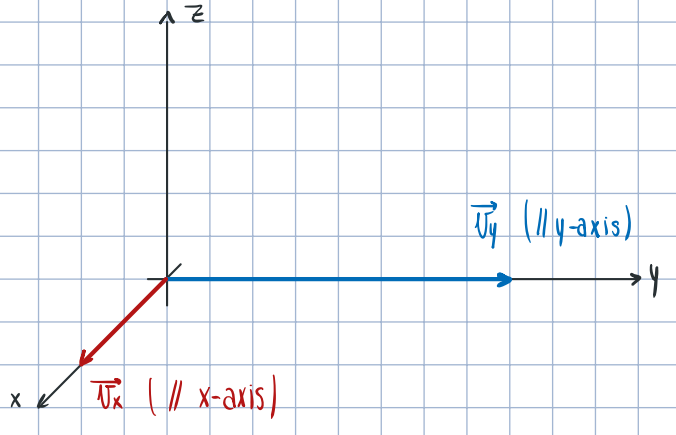
The eigenvalues of $\hat{\Pi}_\varphi$ are

$$\lambda = \begin{cases} 1 & \text{with multiplicity 1 (order of degeneracy)} \\ 0 & \text{with multiplicity } (D-1) \end{cases}$$

For example:

$$\hat{\Pi}_\varphi |\psi\rangle = \begin{cases} |\psi\rangle & \text{for } |\psi\rangle = \alpha|\varphi\rangle \quad (\psi \text{ is the same quantum state of } \varphi) \\ 0 & \text{for } \langle\varphi|\psi\rangle = 0 \quad (\psi \text{ and } \varphi \text{ are orthogonal}) \end{cases}$$

that can be generalized to the euclidian space:



- $\hat{\Pi}_y \vec{v}_y = \vec{v}_y$
- $\hat{\Pi}_y \vec{v}_x = 0$

EXERCISE: Demonstrate that the only possible eigenvalues of an orthogonal projector are 0 and 1.

SOLUTION: By definition of $\hat{\Pi}$ we have the idempotence property:

$$\hat{\Pi}^2 = \hat{\Pi}$$

We can write the eigenvalue function:

$$\hat{\Pi}|\psi\rangle = \lambda|\psi\rangle$$

(λ: eigenvalue; $|\psi\rangle$: eigenket)

$$\hat{\Pi}^2|\psi\rangle = \hat{\Pi}\left(\hat{\Pi}|\psi\rangle\right) = \hat{\Pi}\left(\lambda|\psi\rangle\right) = \lambda\,\hat{\Pi}|\psi\rangle = \lambda\left(\lambda|\psi\rangle\right)$$

$$= \lambda^2|\psi\rangle \quad \text{(I)}$$

→ this is a general property of any operator

In particular for orthogonal projectors:

$$\hat{\Pi}^2|\psi\rangle = \hat{\Pi}|\psi\rangle = \lambda|\psi\rangle \quad \text{(II)}$$

By equating (I) and (II):

$$\lambda^2|\psi\rangle = \lambda|\psi\rangle \qquad \text{for an eigenket } |\psi\rangle \text{ (hence a non-zero vector)}$$

$$\Downarrow$$

$$\lambda^2 = \lambda \longrightarrow \lambda(\lambda - 1) = 0 \longrightarrow \lambda = \begin{cases} 0 \\ 1 \end{cases} \quad \checkmark$$

The "trivial" case of having only 0 eigenvalue is the null operator. The other "trivial" case of having only 1 eigenvalue is the identity operator (rank $\mathcal{R} = D$):

$$\hat{\Pi}_{\mathcal{H}}|\psi\rangle = \hat{1}|\psi\rangle = |\psi\rangle$$

$$\sum_{n=0}^{D-1} 1 \cdot |\varphi_n\rangle\langle\varphi_n| = \hat{1}$$

THEORY OF QUANTUM (PROJECTING) MEASUREMENT

Non-degenerate case: (measurement of an observable with discrete and non-degenerate spectrum)

- discrete: finite or infinite countable dimension of $\mathcal{H}$
- non-degenerate: all eigenvalues are non-degenerate, that is with multiplicity (order of degeneration) equal to 1.

The multiplicity of an eigenvalue is the dimension of the sub-space formed by the corrisponding eigenkets.

$$\hat{A}|\psi\rangle = a|\psi\rangle$$

$$\hat{A}\,|(\alpha|\psi\rangle) = \alpha\,\hat{A}\,|\psi\rangle = a\,(\alpha|\psi\rangle)$$

If $|\psi\rangle$ is eigenket, also $\alpha|\psi\rangle$ is eigenket.

In case of multiplicity g (integer $g \geq 1$) of an eigenvalue, we have g orthonormal eigenkets corresponding to this eigenvalue:

$$\hat{A}\,|\varphi_n\rangle = a\,|\varphi_n\rangle$$

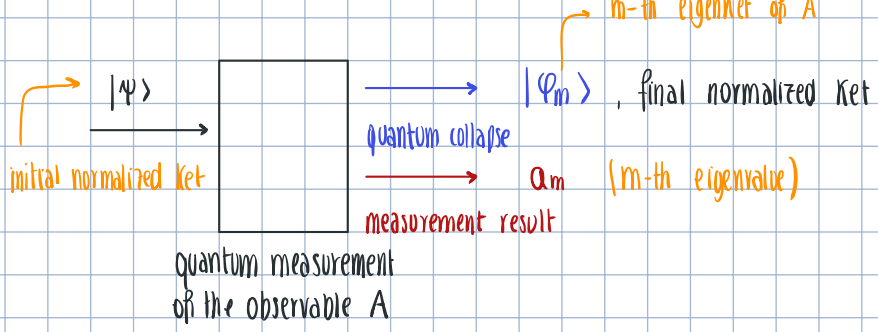
for $\{|\varphi_1\rangle, |\varphi_2\rangle, \dots |\varphi_g\rangle\}$ ⟶ the orthonormal eigenkets

$$\hat{A}\,\Big|\underbrace{\sum_{n=1}^{g}\varphi_n}\Big\rangle = a\,\Big|\sum_{n=1}^{g}\varphi_n\Big\rangle$$

eigenket in a Hilbert sub-space of dimension g

g is the multiplicity of the eigenvalue a

In the non-degenerate case:



Probability (Born's rule):

$$P_m = |\langle\varphi_m|\psi\rangle|^2 = F(\psi, \varphi_m)$$

P_m: squared norm of the orthogonal projection of $|\psi\rangle$ onto $|\varphi_m\rangle$

F: quantum fidelity

Demonstration: The orthogonal projection of $|\psi\rangle$ onto $|\varphi_m\rangle$ is

$$\hat{\Pi}_m\,|\psi\rangle = |\varphi_m\rangle\langle\varphi_m|\psi\rangle$$

$$\|\hat{\Pi}_m\,|\psi\rangle\|^2 = \left(\hat{\Pi}_m\,|\psi\rangle\right)^{\dagger}\left(\hat{\Pi}_m\,|\psi\rangle\right) = \langle\psi|\,\hat{\Pi}_m^{\dagger}\,\hat{\Pi}_m\,|\psi\rangle$$

because the projector is hermitian

$$= \langle\psi|\,\hat{\Pi}_m\,\hat{\Pi}_m|\psi\rangle = \langle\psi|\,\hat{\Pi}_m^2\,|\psi\rangle$$

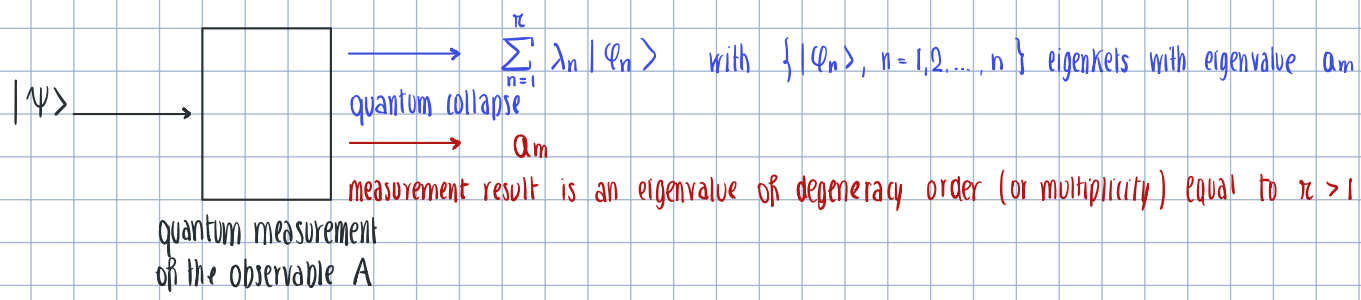
$$= \langle\psi|\,\hat{\Pi}_m|\psi\rangle = \langle\psi|\varphi_m\rangle\langle\varphi_m|\psi\rangle$$

→ for the scalar product the "†" is the same of "*"

$$= \langle\varphi_m|\psi\rangle^{*}\,\langle\varphi_m|\psi\rangle$$

$$= |\langle\varphi_m|\psi\rangle|^2 = P_m \quad \checkmark$$

Degenerate case: (at least one eigenvalue is degenerate)



There is no simple way to generalize the Born's rule, but the probability can be exactly written with the orthogonal projector. The probability of having result of measurement a_m is:

$$P_m = \| \hat{\Pi}_{\Sigma_r} |\psi\rangle \|^2 = \sum_{n=1}^{r} |\langle \varphi_n | \psi \rangle|^2$$

Simultaneous measurement of two observables A and B:

Two observables A, B are simultaneously measurable (for any initial state ψ) if and only if the hermitian operators $\hat{A}, \hat{B}$ commute.

(also known as "compatible observables")

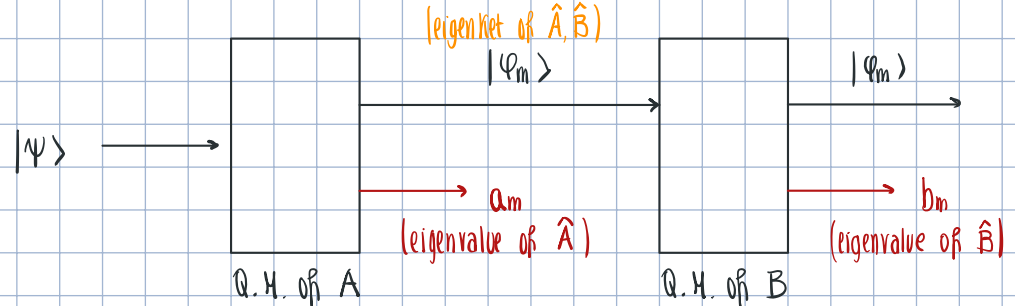
A, B are compatible observables (simultaneously measurable for any initial ψ) $\iff$ Hermitian operator $\hat{A}, \hat{B}$ commute (i.e. $[\hat{A}, \hat{B}] = 0$)

(★)

$\hat{A}, \hat{B}$ have a set of common eigenkets forming an orthonormal basis $\{|\varphi_n\rangle$, with $n = 1,2,\dots,D-1\}$

$$\begin{cases} \hat{A}|\varphi_m\rangle = a_m |\varphi_m\rangle \\ \hat{B}|\varphi_m\rangle = b_m |\varphi_m\rangle \end{cases}$$

The relation (★) can be understood in this way:



After the measurement of $\hat{A}$ and $\hat{B}$ (when $[\hat{A}, \hat{B}] = 0$) there is a quantum collapse (or orthonormal

projection) into a common eigenstate φ_m which is the state with well-defined values a_m and b_m of $\hat{A}$ and $\hat{B}$ (respectlively).

Two observables A, B are not compatible when $[\hat{A}, \hat{B}] \neq 0$

Canonically-conjugate observables (like position and momentum) are not compatible!

Uncertainty principle in general form

$$(\Delta A)_\psi \cdot (\Delta B)_\psi \geq \frac{1}{2} \left| \left\langle \frac{[\hat{A}, \hat{B}]}{i} \right\rangle \right|$$

We can verify that:

$[\hat{A}, \hat{B}]$ = anti-hermitian operator $= i \cdot \hat{C}$

($\hat{A}, \hat{B}$ are hermitian) → $\hat{C}$ hermitian operator

$$[\hat{A}, \hat{B}]^\dagger = -[\hat{A}, \hat{B}]$$

$$\left(\frac{[\hat{A}, \hat{B}]}{i}\right)^\dagger = \frac{[\hat{A}, \hat{B}]}{i}$$

$\hat{x}, \hat{y}, \hat{z}$ are mutually compatible ⟶ it is possible to simultaneously measure x, y, z and hence the position vector $\vec{r} = (x, y, z)$.

$\hat{p}_x, \hat{p}_y, \hat{p}_z$ are compatible ⟶ the momentum vector can be measured

EXERCISE: Verify that

$$[\hat{x}, \hat{y}] = 0$$

$$[\hat{x}, \hat{y}] = \hat{x} \cdot \hat{y} - \hat{y} \cdot \hat{x}$$

We have to verify that

$$\hat{x} \cdot \hat{y} = \hat{y} \cdot \hat{x}$$

SOLUTION: In the position representation:

$$\hat{x} \cdot \hat{y} \, |\psi\rangle \longrightarrow xy \, \psi(x, y, z)$$

$$\hat{y} \cdot \hat{x} \, |\psi\rangle \longrightarrow yx \, \psi(x, y, z)$$

but $xy = yx \longrightarrow xy\,\Psi(x,y,z) = yx\,\Psi(x,y,z)$, so the operators commute:

$$\hat{x}\cdot\hat{y} = \hat{y}\cdot\hat{x}$$

EXERCISE: Verify that

$$[\hat{p}_x, \hat{p}_y] = 0 \longrightarrow \hat{p}_x\cdot\hat{p}_y = \hat{p}_y\cdot\hat{p}_x$$

SOLUTION: In the position representation:

$$\hat{p}_x\,\hat{p}_y\,|\Psi\rangle \longrightarrow \left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial y}\right)\Psi(x,y,z) = -\hbar^2\frac{\partial^2}{\partial x\partial y}\Psi(x,y,z)$$

$$\hat{p}_y\,\hat{p}_x\,|\Psi\rangle \longrightarrow \left(-i\hbar\frac{\partial}{\partial y}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,y,z) = -\hbar^2\frac{\partial^2}{\partial y\partial x}\Psi(x,y,z)$$

but from a mathematical theorem:

$$\frac{\partial^2}{\partial x\partial y} = \frac{\partial^2}{\partial y\partial x}$$

so the operators $\hat{p}_x$ and $\hat{p}_y$ are compatible.

EXERCISE: Verify that $\hat{x}, \hat{p}_x$ are not compatible, that is $[\hat{x}, \hat{p}_x] \neq 0$.

SOLUTION: In the position representation:

$$\hat{x}\,\hat{p}_x\,|\Psi\rangle \longrightarrow x\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,y,z)$$

$$\hat{p}_x\,\hat{x}\,|\Psi\rangle \longrightarrow -i\hbar\frac{\partial}{\partial x}\left(x\,\Psi(x,y,z)\right)$$

$$[\hat{x}, \hat{p}_x]|\Psi\rangle \longrightarrow -i\hbar\,x\frac{\partial}{\partial x}\Psi(x,y,z) + i\hbar\frac{\partial}{\partial x}\left[x\,\Psi(x,y,z)\right] =$$

$$= -i\hbar\left[x\frac{\partial\Psi}{\partial x} - 1\cdot\Psi(x) + x\cdot\frac{\partial\Psi}{\partial x}\right] = i\hbar\,\Psi(x,y,z) \neq 0$$

So the $\hat{x}$ and $\hat{p}_x$ are not compatible.

$$\frac{[\hat{x},\hat{p}_x]}{i} = \hbar\cdot\hat{1} \longrightarrow (\Delta x)(\Delta p_x) \geq \frac{1}{2}\left\langle\frac{[\hat{x},\hat{p}_x]}{i}\right\rangle = \frac{\hbar}{2}$$

UNITARY OPERATORS

We define a linear operator as an UNITARY OPERATOR $\hat{U}$ when its adjoint $\hat{U}^\dagger$ is equal to the inverse $\hat{U}^{-1}$ of the operator.

$$\text{unitary operator } \hat{U} \xleftrightarrow{\text{(def.)}} \hat{U}^\dagger = \hat{U}^{-1} \qquad \left(\text{that is } \hat{U}\cdot\hat{U}^\dagger = \hat{U}\cdot\hat{U}^{-1} = \hat{1}\right)$$

EXERCISE: Verify that any unitary operator is a normal operator.

$\hat{U}$ unitary $\longrightarrow$ normal operator: $\hat{U}\cdot\hat{U}^\dagger = \hat{U}^\dagger\cdot\hat{U}$

SOLUTION: From the definition of unitary operator:

$$\hat{U}\cdot\hat{U}^\dagger = \hat{U}^\dagger\cdot\hat{U} = \hat{1} \quad \checkmark$$

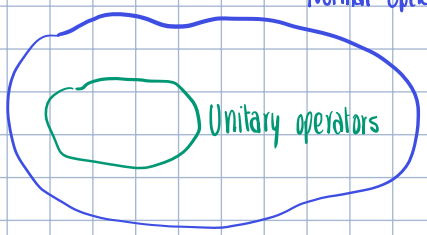
Because any unitary operator is also normal, we can write the unitary operator with the spectral decomposition:

Theorem:

Unitary operator $\hat{U}$ $\xleftrightarrow{(\star)}$ (if and only if) Normal operator having a spectral decomposition:

$$\hat{U} = \sum_n u_n \hat{\Pi}_n = \sum_n u_n |\varphi_n\rangle\langle\varphi_n|$$

with scalar coefficients u_n of modulus equal to one ($|u_n| = 1$) for any $n = 0, 1, 2, \ldots$



moreover we know that u_n are the eigenvalues and $|\varphi_n\rangle$ are the corresponding eigenkets that form a orthonormal basis.

EXERCISE: Demonstrate that

$\hat{U}$ unitary operator $\Longrightarrow$ all the eigenvalues are of unitary modulus: $|u_n| = 1$, $\forall n$

SOLUTION:

$$\hat{U}|\varphi\rangle = u|\varphi\rangle \quad *$$

$$(\hat{U}|\varphi\rangle)^\dagger = (u|\varphi\rangle)^\dagger$$

$$\langle\varphi|\hat{U}^\dagger = \langle\varphi|u^* \quad *$$

↳ it's the dual operator

$$(\langle\varphi|\hat{U}^\dagger)(\hat{U}|\varphi\rangle) = (\langle\varphi|u^*)(u|\varphi\rangle)$$

$$\langle\varphi|\hat{1}|\varphi\rangle = \langle\varphi||u|^2|\varphi\rangle$$

$$\langle\varphi|\varphi\rangle = |u|^2\langle\varphi|\varphi\rangle$$

But $|\varphi\rangle$ is an eigenket and hence is a non-zero vector:

$$\|\varphi\|^2 = \langle\varphi|\varphi\rangle > 0 \quad \Rightarrow \quad |u|^2 = 1 \quad \Rightarrow \quad |u| = 1 \quad \checkmark$$

Demonstration of (☆): Hyp.: $\hat{U} = \sum_n u_n \hat{\Pi}_n = \sum_n e^{i\vartheta_n}|\varphi_n\rangle\langle\varphi_n|$

$e^{i\vartheta_n}$: eigenvalues of unitary modulus

Th.: $\hat{U}^\dagger\cdot\hat{U} = \hat{U}\cdot\hat{U}^\dagger = \hat{1}$

Dem.:

$$\hat{U}^\dagger = \left(\sum_m e^{i\vartheta_m}\hat{\Pi}_m\right)^\dagger = \text{(for the antilinearity of "†")} =$$

$$= \sum_m e^{-i\vartheta_m}\hat{\Pi}_m^\dagger = \text{(orthogonal projectors are hermitian)} =$$

$$= \sum_m e^{-i\vartheta_m}\hat{\Pi}_m$$

(for linearity of $\hat{\Pi}_m$)

$$\hat{U}^\dagger\cdot\hat{U} = \left(\sum_m e^{-i\vartheta_m}\hat{\Pi}_m\right)\left(\sum_n e^{i\vartheta_n}\hat{\Pi}_n\right)$$

$$= \sum_{mn} e^{-i\vartheta_m}e^{i\vartheta_n}\hat{\Pi}_m\cdot\hat{\Pi}_n$$

$$\hat{\Pi}_m\cdot\hat{\Pi}_n = \begin{cases} \hat{\Pi}_m^2 = \hat{\Pi}_m & \text{for } m = n \\ 0 & \text{for } m \neq n \end{cases} = \delta_{mn}\cdot\hat{\Pi}_m$$

In fact: (for the orthonormality of the basis $\{|\varphi_n\rangle,\ n = 0,1,2,\dots\}$)

$$\hat{\Pi}_m\cdot\hat{\Pi}_n = |\varphi_m\rangle\langle\varphi_m|\varphi_n\rangle\langle\varphi_n| = |\varphi_m\rangle\delta_{mn}\langle\varphi_n| = \delta_{mn}|\varphi_m\rangle\langle\varphi_n|$$

$$= \delta_{mn}|\varphi_m\rangle\langle\varphi_m| = \delta_{mn}\cdot\hat{\Pi}_m$$

Hence: (for the closure property)

$$\hat{U}^\dagger\cdot\hat{U} = \sum_{mn} e^{-i\vartheta_m}e^{i\vartheta_n}\delta_{mn}\hat{\Pi}_m = \sum_{n=0}^{D-1}\hat{\Pi}_n = \sum_n |\varphi_n\rangle\langle\varphi_n| = \hat{1} \quad \checkmark$$

In a similar way:

$$\hat{U}\cdot\hat{U}^{\dagger} = \sum_n e^{i\varphi_n}\cdot e^{-i\varphi_n}\hat{\Pi}_n = \dots = \hat{1} \quad \checkmark$$

Theorem: unitary operator $(\hat{U}^{\dagger} = \hat{U}^{-1})$ $\xrightarrow{(*)}$ $\xleftarrow{}$ linear operator conserving the scalar product (and hence the norms)

We can say that unitary operators are the generalization to Hilber spaces of the geometry operations (rotations and reflections) conserving angles and lengths in euclidian spaces.

Demonstration of (*): Hyp.: $\hat{U}$ is unitary operator.

$$|\psi''\rangle = \hat{U}|\psi'\rangle$$

$$|\varphi''\rangle = \hat{U}|\varphi'\rangle$$

Th.: Conservation of the scalar products.

$$\langle\varphi''|\psi''\rangle = \langle\varphi'|\psi'\rangle$$

Dem.: $\langle\varphi''| = |\varphi''\rangle^{\dagger} = \left(\hat{U}|\varphi'\rangle\right)^{\dagger} = \langle\varphi'|\hat{U}^{\dagger}$

$$\langle\varphi''|\psi''\rangle = \langle\varphi'|\underbrace{\hat{U}^{\dagger}\hat{U}}_{=\hat{1}}|\psi'\rangle = \langle\varphi'|\hat{1}|\psi'\rangle = \langle\varphi'|\psi'\rangle \quad \checkmark$$

In particular:

$$\|\hat{U}|\psi\rangle\| = \||\psi\rangle\|$$

being

$$\|\hat{U}|\psi\|^2 = \left(\hat{U}|\psi\right)^{\dagger}\cdot\left(\hat{U}|\psi\rangle\right) = \langle\psi|\hat{U}^{\dagger}\cdot\hat{U}|\psi\rangle = \||\psi\rangle\|^2 \quad \checkmark$$

We can say that:

unitary operator $\Longleftrightarrow$ linear operator transforming an orthonormal basis $\{|\varphi_n\rangle,\ n = 0,1,2,\dots\}$ into another orthonormal basis $\{|\tilde{\varphi}_n\rangle = \hat{U}|\varphi_n\rangle,\ n = 0,1,2,\dots\}$

It is obvious that the orthonormality of the basis is preserved by applying $\hat{U}$.

$$\langle\varphi_m|\varphi_n\rangle = \delta_{mn}$$

$$\langle \tilde{\varphi}_m | \tilde{\varphi}_n \rangle = \langle \varphi_m | \hat{U}^\dagger \hat{U} | \varphi_n \rangle = \langle \varphi_m | \hat{1} | \varphi_n \rangle = \langle \varphi_m | \varphi_n \rangle = \delta_{mn}$$

An unitary operator $\hat{U}$ is represented in a given orthonormal basis by an unitary matrix U, that is a matrix with inverse matrix U^{-1} equal to the conjugate transpose matrix $U^\dagger$.

The matrix coefficients of $\hat{U}$ are:

$$U_{mn} = \langle \varphi_m | \hat{U} | \varphi_n \rangle$$

The inverse matrix shows coefficients:

$$U_{mn}^{-1} = \langle \varphi_m | \hat{U}^{-1} | \varphi_n \rangle = \langle \varphi_m | \hat{U}^\dagger | \varphi_n \rangle = U_{mn}^\dagger = U_{nm}^*$$

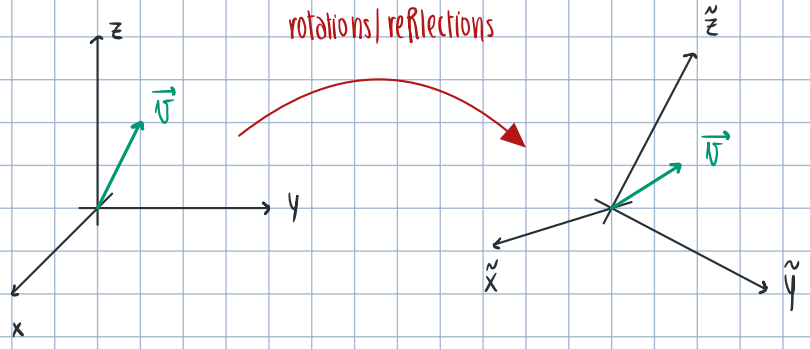
in a given orthonormal basis $\{ | \varphi_n \rangle, \; n = 0, 1, 2, \dots \}$

$\hat{U}$ unitary operator $\iff$ unitary matrix U in a given orthonormal basis $\iff$ the inverse matrix is the conjugate transpose matrix:

$$U_{mn}^{-1} = U_{nm}^*$$

$\Updownarrow$

matrix with orthonormal columns (raws)



fixed vector → scalar coefficients depends on the cartesian reference

$$\{ | \varphi_n \rangle, \; n = 0, 1, 2, \dots \} \xrightarrow{\text{unitary operator } \hat{U}} \{ | \tilde{\varphi}_n \rangle, \; n = 0, 1, 2, \dots \}$$

fixed ket $|\psi\rangle \implies$ scalar coefficients $\lambda_n = \langle \varphi_n | \psi \rangle$ depending on the basis

$$|\psi\rangle = \sum_n | \varphi_n \rangle \langle \varphi_n | \psi \rangle = \sum_n \lambda_n | \varphi_n \rangle \quad \xleftrightarrow{\text{matrix representation}} \quad \begin{bmatrix} \vdots \\ \lambda_n \\ \vdots \end{bmatrix} \text{ column vector}$$

In the new basis $\{ |\tilde{\varphi}_m\rangle,\ m = 0,1,2,\dots \}$ the same ket $|\psi\rangle$ is represented by the column vector:

$$\begin{bmatrix} \vdots \\ \tilde{\lambda}_m = \langle \tilde{\varphi}_m | \psi \rangle \\ \vdots \end{bmatrix}$$

Calculate the relation between $\{\tilde{\lambda}_m\}$ and $\{\lambda_n\}$:

$$\tilde{\lambda}_m = \langle \tilde{\varphi}_m | \psi \rangle$$

but $\langle \tilde{\varphi}_m | = |\tilde{\varphi}_m\rangle^\dagger = |\hat{U}|\varphi_m\rangle)^\dagger = \langle \varphi_m | \hat{U}^\dagger$. Hence:

$$\tilde{\lambda}_m = \langle \varphi_m | \hat{U}^\dagger | \psi \rangle = \langle \varphi_m | \hat{U}^\dagger \cdot \hat{1} | \psi \rangle = \langle \varphi_m | \hat{U}^\dagger \cdot \sum_n \lambda_n | \varphi_n \rangle = \sum_n \lambda_n \langle \varphi_m | \hat{U}^\dagger | \varphi_n \rangle$$

$$= \sum_n \lambda_n \cdot U^\dagger_{mn} = \sum_n U^\dagger_{mn} \cdot \lambda_n = \sum_n U^{-1}_{mn} \cdot \lambda_n$$

$$\boxed{\tilde{\lambda}_m = \sum_n U^{-1}_{mn} \cdot \lambda_n}$$

in matrix form →

$$\begin{bmatrix} \vdots \\ \tilde{\lambda}_m \\ \vdots \end{bmatrix} = \begin{bmatrix} \cdots & \vdots & \cdots \\ & U^{-1}_{mn} & \\ & \vdots & \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ \lambda_n \\ \vdots \end{bmatrix}$$

or equivalently

$$\begin{bmatrix} \vdots \\ \tilde{\lambda}_m \\ \vdots \end{bmatrix} = \begin{bmatrix} \cdots & \vdots & \cdots \\ & U^\dagger_{mn} & \\ & \vdots & \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ \lambda_n \\ \vdots \end{bmatrix}$$

with $U^{-1}_{mn} = U^\dagger_{mn} = U^*_{nm}$

Consider now a linear operator $\hat{A}$ represented in an orthonormal basis $\{ |\varphi_n\rangle,\ n = 0,1,2,\dots \}$ by matrix coefficients:

$$A_{mn} = \langle \varphi_m | \hat{A} | \varphi_n \rangle$$

Now we want to calculate the matrix coefficients in another orthonormal basis $\{ |\tilde{\varphi}_n\rangle$, with $n = 0,1,2,\dots \}$:

$$\tilde{A}_{mn} = \langle \tilde{\varphi}_m | \hat{A} | \tilde{\varphi}_n \rangle \qquad \text{with } |\tilde{\varphi}_n\rangle = \hat{U}|\varphi_n\rangle$$

$$\tilde{A}_{mn} = \langle \tilde{\varphi}_m | \hat{A} | \tilde{\varphi}_n \rangle = \langle \tilde{\varphi}_m | \big(\hat{1}\big) \cdot \hat{A} \cdot \big(\hat{1}\big) | \tilde{\varphi}_n \rangle = \langle \tilde{\varphi}_m | \Big(\sum_h |\varphi_h\rangle\langle\varphi_h|\Big) \cdot \hat{A} \cdot \Big(\sum_k |\varphi_k\rangle\langle\varphi_k|\Big) \tilde{\varphi}_n \rangle =$$

(closure property; closure property)

$$= \sum_{mn} \langle \tilde{\varphi}_m | \varphi_h \rangle \langle \varphi_h | \hat{A} | \varphi_k \rangle \langle \varphi_k | \tilde{\varphi}_n \rangle$$

$$= \sum_{mn} \langle \varphi_m | \hat{U}^\dagger | \varphi_h \rangle \langle \varphi_h | \hat{A} | \varphi_k \rangle \langle \varphi_k | \hat{U} | \varphi_n \rangle$$

$$= \sum_{mn} U^\dagger_{mh} \cdot A_{hk} \cdot U_{kn}$$

$$\begin{bmatrix} \vdots \\ \cdots \tilde{A}_{mn} \cdots \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \cdots U^{+}_{mh} \cdots \\ \vdots \end{bmatrix} \begin{bmatrix} \vdots \\ \cdots A_{hk} \cdots \\ \vdots \end{bmatrix} \begin{bmatrix} \vdots \\ \cdots U_{kn} \cdots \\ \vdots \end{bmatrix} \qquad \text{with} \quad U^{+}_{mh} = U^{-1}_{mh} = U^{*}_{hm}$$

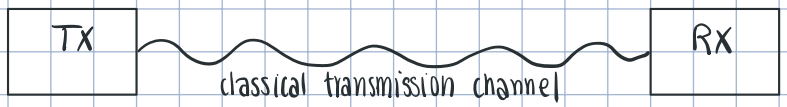
QUBITS

The "classical bit" is described by a classical physical system that can assume only two states:

- bit 0
- bit 1

For example:

The bit can be transmitted. For example:

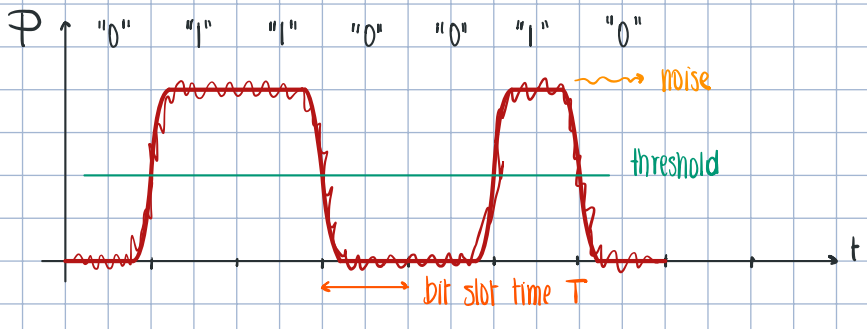


Transmitted bit sequence:
$\cdots 01001101 \cdots$

Recieved bit sequence
$\cdots 01011100 \cdots$ (with some errors) → due to noise

After error correction, the recieved bit sequence is identical to the transmitted one.

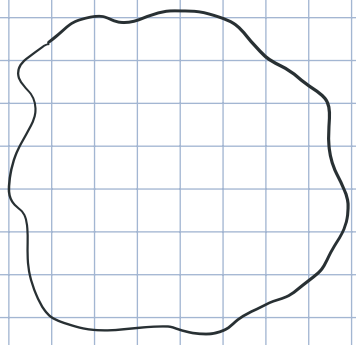
Example: in optical communications, the classical bits are implemented as ON-OFF light pulses



bit rate $\triangleq f_B = 1/T \ [s^{-1}]$

The classical bit can be also described by a deterministic logic (or boolean) variable assuming the values "true" or "false".

In quantum information and computing the basic element of information is the quantum bit (named "QUBIT") instead of the classical bit.



Quantum physical system obtained as superposition of two basis orthogonal quantum states:

$|0\rangle$ and $|1\rangle$

generating an Hilbert space of dimension $D = 2$.

The qubit is the quantum state of a physical quantum system described by a 2-D Hilbert space, expressed by a linear superposition:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

generic qubit; first basis qubit; second basis qubit

Orthonormal basis for qubit Hilbert space:

$$\{|\varphi_n\rangle,\ n = 0,1\} = \{|\varphi_0\rangle \equiv |0\rangle,\ |\varphi_1\rangle \equiv |1\rangle\}$$

So α and β are the scalar (complex) coefficients of the expansion of the qubit $|\psi\rangle$.

qubit $|\psi\rangle$ $\longleftrightarrow$ representation in the "computational basis" $\{|0\rangle, |1\rangle\}$

$$\begin{bmatrix} \langle\varphi_0|\psi\rangle = \langle 0|\psi\rangle = \alpha \\ \langle\varphi_1|\psi\rangle = \langle 1|\psi\rangle = \beta \end{bmatrix}$$

$\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ represents the qubit.

EXERCISE: Calculate $\langle 0|\psi\rangle$.

SOLUTION:

$$\langle 0|\psi\rangle = \langle 0|\left(\alpha|0\rangle + \beta|1\rangle\right) = \langle 0|\alpha|0\rangle + \langle 0|\beta|1\rangle =$$

$$= \alpha\langle 0|0\rangle + \beta\langle 0|1\rangle$$

But for the orthonormality of the basis ($\langle\varphi_m|\varphi_n\rangle = \delta_{mn}$):

$$\Rightarrow \quad \alpha\langle 0|0\rangle + \beta\langle 0|1\rangle = \alpha\cdot 1 + \beta\cdot 0 = \alpha$$

The normalization condition for qubit is:

$$|\alpha|^2 + |\beta|^2 = 1$$

Demonstration:

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

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$\langle\psi| = |\psi\rangle^\dagger = \alpha^*\langle 0| + \beta^*\langle 1|$$

$$\Rightarrow \quad \langle\psi|\psi\rangle = (\alpha^*\langle 0| + \beta^*\langle 1|)(\alpha|0\rangle + \beta|1\rangle)$$

$$= \alpha^*\alpha \underbrace{\langle 0|0\rangle}_{=1} + \alpha^*\beta \underbrace{\langle 0|1\rangle}_{=0} + \beta^*\alpha \underbrace{\langle 1|0\rangle}_{=0} + \beta^*\beta \underbrace{\langle 1|1\rangle}_{=1}$$

$$= |\alpha|^2 + |\beta|^2$$

The norm of the qubit is thus:

$$\| \psi \| = \sqrt{|\alpha|^2 + |\beta|^2}$$

Example: demonstration using matrix algebra.

QUBIT
- bra: $|\psi\rangle \longleftrightarrow \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$
- ket: $\langle\psi| \longleftrightarrow \begin{bmatrix} \alpha \\ \beta \end{bmatrix}^\dagger = \begin{bmatrix} \alpha^* & \beta^* \end{bmatrix}$

$$\| \psi \|^2 = \langle\psi|\psi\rangle = \begin{bmatrix} \alpha^* & \beta^* \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha^*\alpha + \beta^*\beta = |\alpha|^2 + |\beta|^2$$

SINGLE-QUBIT QUANTUM GATES

$|\psi_{in}\rangle \longrightarrow$ unitary operator $\hat{U} \longrightarrow |\psi_{out}\rangle$

$$|\psi_{out}\rangle = \hat{U}|\psi_{in}\rangle$$

$$\begin{bmatrix} \alpha_{in} \\ \beta_{in} \end{bmatrix} \qquad \begin{bmatrix} \alpha_{out} \\ \beta_{out} \end{bmatrix}$$

$$\begin{bmatrix} \alpha_{out} \\ \beta_{out} \end{bmatrix} = \begin{bmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{bmatrix} \cdot \begin{bmatrix} \alpha_{in} \\ \beta_{in} \end{bmatrix}$$

$$U_{mn} = \langle \varphi_m | \hat{U} | \varphi_n \rangle \qquad \text{with } m, n = 0, 1 \quad \text{(for the qubits)}$$

$$\begin{cases} U_{00} = \langle 0|\hat{U}|0\rangle \\ U_{01} = \langle 0|\hat{U}|1\rangle \\ U_{10} = \langle 1|\hat{U}|0\rangle \\ U_{11} = \langle 1|\hat{U}|1\rangle \end{cases} \longrightarrow$$

matrix coefficients of the unitary operator $\hat{U}$ describing a quantum gate in the computational basis $\{|0\rangle, |1\rangle\}$

$$\begin{cases} \alpha_{out} = U_{00}\cdot\alpha_{in} + U_{01}\cdot\beta_{in} \\ \beta_{out} = U_{10}\cdot\alpha_{in} + U_{11}\cdot\beta_{in} \end{cases}$$

Example:

$|0\rangle \longrightarrow \begin{bmatrix}1\\0\end{bmatrix} \longrightarrow \boxed{\hat{U}} \longrightarrow \hat{U}|0\rangle$

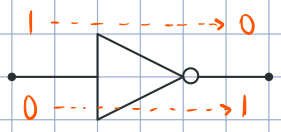
$$\begin{bmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix} U_{00} \\ U_{10} \end{bmatrix}$$

is the first column of the matrix!

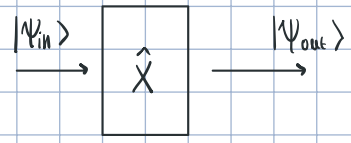
$|1\rangle \longrightarrow \begin{bmatrix}0\\1\end{bmatrix} \longrightarrow \boxed{\hat{U}} \longrightarrow \hat{U}|1\rangle = \begin{bmatrix} U_{01} \\ U_{11} \end{bmatrix}$

second column of the matrix

"Quantum - NOT" gate (PAULI - X GATE)



classical NOT



quantum NOT

Characteristic action of $\hat{X}$ on the basis qubits:

$$\begin{cases} |0\rangle \xrightarrow{\hat{X}} |1\rangle \\ |1\rangle \xrightarrow{\hat{X}} |0\rangle \end{cases}$$

A linear operator is completely characterized by its action on the basis vectors (i.e. by the matrix coefficients).

$$\begin{bmatrix}1\\0\end{bmatrix} \xrightarrow{U} \begin{bmatrix}0\\1\end{bmatrix} \qquad \text{first column of } X$$

$$\begin{bmatrix}0\\1\end{bmatrix} \xrightarrow{U} \begin{bmatrix}1\\0\end{bmatrix} \qquad \text{second column of } X$$

$$X = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} \longrightarrow \text{Pauli-X matrix}$$

$$\begin{bmatrix}\alpha_{out}\\ \beta_{out}\end{bmatrix} = X \cdot \begin{bmatrix}\alpha_{in}\\ \beta_{in}\end{bmatrix} = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} \cdot \begin{bmatrix}\alpha_{in}\\ \beta_{in}\end{bmatrix} = \begin{bmatrix}\beta_{in}\\ \alpha_{in}\end{bmatrix}$$

Pauli's operator (definition): unitary and hermitian operator with eigenvalues ± 1 (acting on qubits, so in a 2-D Hilbert space).

EXERCISE: Verify that X is unitary and hermitian.

SOLUTION: ① X is unitary because it is a mapping between orthonormal basis. In fact we have:

$$X^\dagger = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}^\dagger = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} = X$$

$$X^\dagger \cdot X = X \cdot X = X^2$$

$$X \cdot X^\dagger = X \cdot X = X^2$$

and:

$$X^2 = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} \cdot \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} = I$$

hence:

$$X^\dagger \cdot X = X \cdot X^\dagger = I \rightsquigarrow \text{identity matrix}$$

$$X^{-1} = X^\dagger \Rightarrow X \text{ is unitary.}$$

We also have

$$X^\dagger = X \Rightarrow X \text{ is hermitian (observable)}$$

The eigenstates of $\hat{X}$ are the orthonormalized states:

$$\begin{cases} |+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \\ |-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) \end{cases}$$

EXERCISE: Verify that $\langle +|-\rangle = 0$ and $\langle +|+\rangle = \langle -|-\rangle = 1$.

SOLUTION:

$$\langle +| = |+\rangle^{\dagger} = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)^{\dagger} = \frac{1}{\sqrt{2}}\left(\langle 0| + \langle 1|\right)$$

$$\langle +|-\rangle = \frac{1}{\sqrt{2}}\left(\langle 0| + \langle 1|\right) \cdot \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) =$$

$$= \frac{1}{2}\left(\langle 0|0\rangle - \langle 0|1\rangle + \langle 1|0\rangle - \langle 1|1\rangle\right)$$

$$= \frac{1}{2}\left(|1 - 1\right) = 0 \qquad \text{(in bra-ket notation)}$$

In matrix algebra:

$$|+\rangle \longleftrightarrow \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$|-\rangle \longleftrightarrow \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

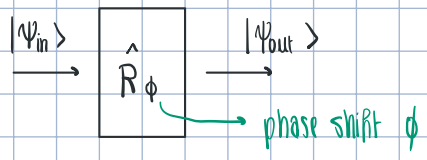
$$\langle +|-\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}^{\dagger} \cdot \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{2}\left(1 - 1\right) = 0$$

In fact we have:

$$\begin{cases} \hat{X}|+\rangle = |+\rangle & \text{(eigenvalue } +1\text{)} \\ \hat{X}|-\rangle = -|-\rangle & \text{(eigenvalue } -1\text{)} \end{cases}$$

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ 1 \end{bmatrix} = -\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Phase shift gate



$$\begin{cases} \hat{R}_\phi |0\rangle = |0\rangle \\ \hat{R}_\phi |1\rangle = e^{i\phi} |1\rangle \end{cases}$$

In this case the eigenkets are $\{|0\rangle, |1\rangle\}$ with eigenvalues $\{1, e^{i\phi}\}$.

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix} \xrightarrow{\hat{R}_\phi} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{(first column of } R_\phi\text{)}$$

$$\begin{bmatrix} 0 \\ 1 \end{bmatrix} \xrightarrow{\hat{R}_\phi} e^{i\phi} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \text{(second column of } R_\phi\text{)}$$

$$R_\phi = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$$

Diagonal matrix because the basis qubits $|0\rangle, |1\rangle$ are eigenstates of $\hat{R}_\phi$.

In the particular case of $\phi = \pi$ we obtain the PAULI-Z GATE

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \text{(diagonal matrix with eigenvalues } \pm 1\text{, and also hermitian)}$$

$$R_\phi^\dagger = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}^\dagger = \begin{bmatrix} 1 & 0 \\ 0 & e^{-i\phi} \end{bmatrix}$$

In general $R_\phi^\dagger \neq R_\phi$ (not hermitian), except for

$$\phi = 0 \quad \Rightarrow \quad R_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$$

$$\phi = \pi \quad \Rightarrow \quad R_\pi = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = Z$$

- S-GATE : $\hat{S} = \hat{R}_{\pi/2}$

$$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$$

- **T-GATE:** $\hat{T} = \hat{R}_{\pi/4}$

$$T = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$$

- **PAULI - Y GATE:**

$$\begin{cases} |0\rangle \xrightarrow{\hat{y}} i|1\rangle & i\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ i \end{bmatrix} \\ |1\rangle \xrightarrow{\hat{y}} -i|0\rangle & -i\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -i \\ 0 \end{bmatrix} \end{cases}$$

$$Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Y is both unitary and hermitian with eigenvalues ± 1

The eigenkets of $\hat{y}$ are:

$$\begin{cases} |i\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + i|1\rangle\right) & \text{with eigenvalue } +1 \\ |-i\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - i|1\rangle\right) & \text{with eigenvalue } -1 \end{cases}$$

In fact we have

$$\hat{y}|\pm i\rangle = \frac{1}{\sqrt{2}}\hat{y}\left(|0\rangle \pm i|1\rangle\right) \overset{\text{matrix representation}}{=} \frac{1}{\sqrt{2}} Y \cdot \begin{bmatrix} 1 \\ \pm i \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\cdot\begin{bmatrix} 1 \\ \pm i \end{bmatrix}$$

$$= \frac{1}{\sqrt{2}}\begin{bmatrix} \pm 1 \\ i \end{bmatrix} = \underset{\text{eigenvalues } \pm 1}{(\pm)} \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ \pm i \end{bmatrix}$$

A normal operator can also be defined by its spectral decomposition, that is knowing its eigenvalues and eigenvectors.

EXERCISE: calculate the matrix representing the Pauli - Y gate, using the spectral decomposition.

SOLUTION: The Pauli - Y gate has eigenkets:

$$|\pm i\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \pm i|1\rangle\right)$$

with respective eigenvalues ± 1, so its spectral decomposition is:

$$\hat{Y} = +1 \cdot \hat{\Pi}_{|i\rangle} - 1 \cdot \hat{\Pi}_{|-i\rangle}$$

eigenvalues — orthogonal projector onto $|i\rangle$ and $|-i\rangle$

$$= |i\rangle\langle i| - |-i\rangle\langle -i|$$

In terms of matrix we have:

$$Y = \hat{\Pi}_{|i\rangle} - \hat{\Pi}_{|-i\rangle}$$

Where $\hat{\Pi}_{|i\rangle} = |i\rangle\langle i|$ is represented by the matrix:

$$\Pi_{|i\rangle} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix} \cdot \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -i \end{bmatrix}$$

column vector representing the ket $|i\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + i|1\rangle\right)$

raw vector representing the bra $\langle i| = |i\rangle^{+} = \frac{1}{\sqrt{2}}\left(\langle 0| - i\langle 1|\right)$

$$\Pi_{|i\rangle} = \frac{1}{2}\begin{bmatrix} 1 \\ i \end{bmatrix} \cdot \begin{bmatrix} 1 & -i \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix}$$

(raw-by-column) matrix product

The orthogonal projector onto the other eigenket $|-i\rangle$ of $\hat{Y}$:

$$\hat{\Pi}_{|-i\rangle} = |-i\rangle\langle -i|$$

is represented by the matrix:

$$\Pi_{|-i\rangle} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix} \cdot \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & i \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}$$

We remark that the sum of the two matrices $\Pi_{|i\rangle}$ and $\Pi_{|-i\rangle}$ is the identity matrix.

$$\Pi_{|i\rangle} + \Pi_{|-i\rangle} = \frac{1}{2}\begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$$

This is a general property for the sum of the orthogonal projectors onto each vector of an orthonormal basis $\{|\varphi_n\rangle\}_{n=0,1,2,\dots,D-1}$

According to the closure property:

$$\sum_{n=0}^{D-1} \hat{\Pi}_{|\varphi_n\rangle} = \sum_{n=0}^{D-1} |\varphi_n\rangle\langle\varphi_n| = \hat{1}$$

In case of the Hilbert space of qubits (dimension $D = 2$) we have:

$$\hat{\Pi}_{|\varphi_0\rangle} + \hat{\Pi}_{|\varphi_1\rangle} = |\varphi_0\rangle\langle\varphi_0| + |\varphi_1\rangle\langle\varphi_1| = \hat{1}$$

Hence it is also possible to calculate the second projector matrix, after calculating the first one, as:

$$\Pi_{|-i\rangle} = I - \hat{\Pi}_{|i\rangle} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}$$

The matrix of the Pauli-Y gate can be then obtained from the spectral decomposition:

$$Y = \Pi_{|i\rangle} - \Pi_{|-i\rangle} = \frac{1}{2}\begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

From this matrix we obtain the rule of application of Pauli-Y gate on the computational basis:

$$\begin{cases} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \xrightarrow{Y} \begin{bmatrix} 0 \\ i \end{bmatrix} \\ \begin{bmatrix} 0 \\ 1 \end{bmatrix} \xrightarrow{Y} \begin{bmatrix} -i \\ 0 \end{bmatrix} \end{cases}$$

first column of matrix Y

second column of matrix Y

That is, in bra-ket notation:

$$\begin{cases} \hat{Y}|0\rangle = i|1\rangle \\ \hat{Y}|1\rangle = -i|0\rangle \end{cases}$$

NOTE: The matrix representing a Pauli gate in an orthonormal basis (for example the computational basis) is both hermitian and unitary. It is possible to make a quick check of these properties in terms of the matrix coefficients.

Let us consider a 2×2 matrix (representing a linear operator acting on qubits):

$$A = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix}$$

The adjoint matrix (or hermitian conjugate, or conjugate transpose matrix) is

$$A^{+} = \begin{bmatrix} A_{00}^{*} & A_{10}^{*} \\ A_{01}^{*} & A_{11}^{*} \end{bmatrix}$$

A is a hermitian (or self-adjoint) matrix by definition when $A = A^{+}$ that is:

$$\begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} = \begin{bmatrix} A_{00}^{*} & A_{10}^{*} \\ A_{01}^{*} & A_{11}^{*} \end{bmatrix}$$

meaning that the diagonal elements A_{00}, A_{11} must be real:

$$\begin{cases} A_{00} = A_{00}^{*} \\ A_{11} = A_{11}^{*} \end{cases}$$

while the out-of-diagonal elements A_{01}, A_{10} must be complex conjugated

$$\begin{cases} A_{01} = A_{10}^{*} \\ A_{10} = A_{01}^{*} \end{cases}$$

In case of Pauli-Y gate this property of coefficients is verified

$$Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

the out-of-diagonal elements are complex conjugate

the diagonal elements are real

NOTE: A matrix

$$U = \begin{bmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{bmatrix}$$

is a unitary matrix by definition when the adjoint matrix $U^{\dagger}$ is the inverse matrix U^{-1}, that is:

$$U \cdot U^{\dagger} = U \cdot U^{-1} = I$$

Moreover, the unitary matrices represent in an orthonormal basis the unitary operators which have the characteristic property of performing transformations (or mappings) between orthonormal basis.

Hence the columns (which are image vectors of an orthonormal basis) must form another orthonormal basis, that is a unitary matrix is characterized by having orthonormal columns (and also raws).

The conditions for having a 2×2 unitary matrix (representing a quantum gate acting on a single qubits) are:

$$\begin{cases} |U_{00}|^2 + |U_{10}|^2 = 1 & \text{normalized first column} \\ |U_{01}|^2 + |U_{11}|^2 = 1 & \text{normalized second column} \\ U_{00}^* \cdot U_{01} + U_{10}^* \cdot U_{11} = 0 & \text{orthogonal columns} \end{cases}$$

or equivalently:

$$\begin{cases} |U_{00}|^2 + |U_{01}|^2 = 1 & \text{normalized first raw} \\ |U_{10}|^2 + |U_{11}|^2 = 1 & \text{normalized second raw} \\ U_{00}^* \cdot U_{10} + U_{01}^* \cdot U_{11} = 0 & \text{orthogonal raws} \end{cases}$$

It is sufficient to check the columns (or the raws) and in case of orthonormality of the columns, also if the raws are orthonormal (or viceversa)

In fact, if U is unitary also $U^{-1} = U^\dagger$ is unitary, so the orthonormality condition applies for both columns and raws.

EXERCISE: Verify that the columns of Pauli-Y matrix are orthonormal:

$$Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

SOLUTION: Squared norm of the first column $\left\| \begin{bmatrix} 0 \\ i \end{bmatrix} \right\|^2 = |0|^2 + |i|^2 = 0 + 1 = 1$ ✓

Squared norm of the second column $\left\| \begin{bmatrix} -i \\ 0 \end{bmatrix} \right\|^2 = |-i|^2 + |0|^2 = 1 + 0 = 1$ ✓

Scalar product between columns $\begin{bmatrix} 0 \\ i \end{bmatrix}^{+} \cdot \begin{bmatrix} -i \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & -i \end{bmatrix} \cdot \begin{bmatrix} -i \\ 0 \end{bmatrix} = 0(-i) + (-i) \cdot 0 = 0$ ✓

HADAMARD GATE $\hat{H}$

$|0\rangle \xrightarrow{\hat{H}} |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ → column vector $\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$

orthonormal basis ↕ orthonormal basis

$|1\rangle \xrightarrow{\hat{H}} |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ → column vector $\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$

Representing matrix (in the computational basis):

$$H = \frac{1}{\sqrt{2}}\cdot\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$

The Hadamard gate is another Pauli's gate (hermitian, unitary, with eigenvalues ± 1). In general:

$\hat{H} = \hat{H}^{\dagger}$ (hermitian operator)

$\hat{H}^{-1} = \hat{H}^{\dagger}$ (unitary operator)

Pauli's operator $\Rightarrow$ $\hat{H} = \hat{H}^{-1}$

$(\hat{X}, \hat{X}^{-1}, \dots)$ involutory property of Pauli's operator

$\hat{H}^2 = \hat{H}\cdot\hat{H} = \hat{H}\cdot\hat{H}^{-1} = \hat{1}$

From the involutory property:

$\lambda^2 = 1$

so the eigenvalues: $\lambda = \pm 1$

{ Unitary operators $\Rightarrow$ eigenvalues $e^{i\theta}$ of modulus 1
Hermitian operators $\Rightarrow$ real eigenvalues } $\Rightarrow$ eigenvalues ± 1

We can write:

$$\hat{H} = \frac{\hat{X}+\hat{Z}}{\sqrt{2}}$$

where $X = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$ (quantum not gate) and $Z = \begin{bmatrix}1 & 0\\ 0 & e^{i\pi}\end{bmatrix} = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$ (R_π)

$$= \frac{1}{\sqrt{2}}\cdot\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$

Theorem: The four operators $\{\hat{X}, \hat{Y}, \hat{Z}, \hat{1}\}$ form a basis for the vectorial space of the linear operators acting on qubits: (that is a 2×2 matrices)

$$\hat{A} = a_0 \cdot \hat{1} + a_1 \cdot \hat{X} + a_2 \cdot \hat{Y} + a_3 \cdot \hat{Z} \qquad \text{(4 dimensional vectorial space)}$$

$$= \sum_{n=0}^{3} a_n \cdot \hat{\sigma}_n$$

where:

$$\begin{cases} \hat{\sigma}_0 = \hat{1} \\ \hat{\sigma}_1 = \hat{X} \\ \hat{\sigma}_2 = \hat{Y} \\ \hat{\sigma}_3 = \hat{Z} \end{cases}$$

Theorem: A linear operator $\hat{A}$ acting on qubits (that is acting on a bidimensional Hilbert space) is hermitian (observable) if and only if

$$\hat{A} = \sum_{n=0}^{3} a_n \hat{\sigma}_n \qquad \text{with all real } a_n$$

Theorem: A linear operator $\hat{\sigma}_{\vec{v}}$ acting on qubits is a Pauli's operator if and only if ($\vec{v}$: 3-D vector $\vec{v} = (v_1, v_2, v_3)$)

$$\hat{\sigma}_{\vec{v}} = \vec{v} \cdot \vec{\hat{\sigma}}$$

$$= \sum_{n=1}^{3} v_n \cdot \hat{\sigma}_n = v_1 \cdot \hat{X} + v_2 \cdot \hat{Y} + v_3 \cdot \hat{Z}$$

with $\vec{v}$ real and normalized 3-D vector

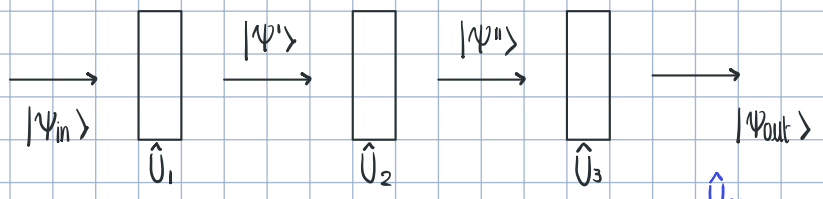
$$v_1^2 + v_2^2 + v_3^2 = 1$$

Example: For Hadamar operator we have:

$$\begin{cases} v_1 = 1/\sqrt{2} \\ v_2 = 0 \\ v_3 = 1/\sqrt{2} \end{cases}$$

$$H = \frac{X+Z}{\sqrt{2}}$$

Any quantum circuit acting on single qubits can be obtained as the cascade of quantum gates (unitary operators):



$$|\psi_{out}\rangle = \hat{U}_3 |\psi''\rangle = \hat{U}_3 \cdot \hat{U}_2 |\psi'\rangle = \underbrace{\hat{U}_3 \cdot \hat{U}_2 \cdot \hat{U}_1}_{\hat{U}_{eq}} |\psi_{in}\rangle$$

The cascade of quantum gates is equivalent to a single gate equal to the product in reversed order:

$$|\psi_{out}\rangle = \hat{U}_{eq} |\psi_{in}\rangle \qquad \text{with} \quad \hat{U}_{eq} = \hat{U}_n \cdot \hat{U}_{n-1} \cdot \hat{U}_{n-2} \cdot \ldots \cdot \hat{U}_2 \cdot \hat{U}_1$$

The product of unitary operators is still unitary.

BLOCH'S SPHERE REPRESENTATION

A generic qubit can be seen as superposition of two orthonormal basis qubits (for example $|0\rangle, |1\rangle$):

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Normalization condition for qubits:

$$|\alpha|^2 + |\beta|^2 = 1$$

$|\psi\rangle$ (qubit) $\longrightarrow$ $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ (column vector) $\xrightarrow{\text{in case of normalization}}$

$\phi_1 = \arg \alpha$, $\phi_2 = \arg \beta$

$$\begin{bmatrix} e^{i\phi_1} |\alpha| \\ e^{i\phi_2} |\beta| \end{bmatrix} = \begin{bmatrix} e^{i\phi_1} \cos\left(\frac{\vartheta}{2}\right) \\ e^{i\phi_2} \sin\left(\frac{\vartheta}{2}\right) \end{bmatrix} =$$

α and β like the sine and cosine of the same thing that we call $\vartheta/2$.

$$= e^{i\phi_1} \begin{bmatrix} \cos(\vartheta/2) \\ e^{i(\phi_2 - \phi_1)} \sin(\vartheta/2) \end{bmatrix}$$

Representation of a normalized qubit

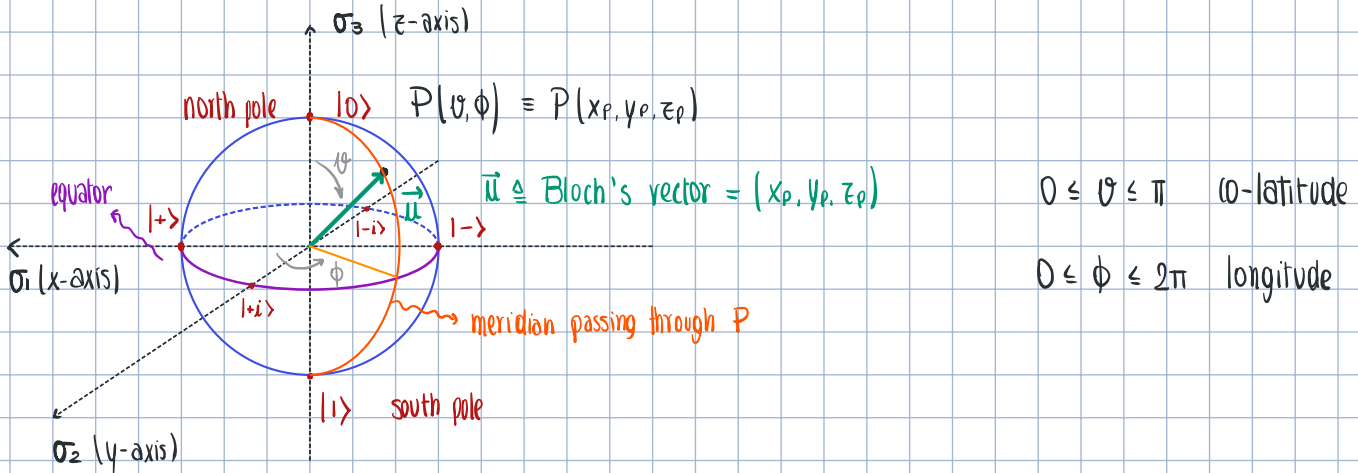
$$= e^{i\phi_1} \begin{bmatrix} \cos(\vartheta/2) \\ e^{i\phi} \sin(\vartheta/2) \end{bmatrix}$$

We can impose $\phi_1 = 0$ (the qubit is defined as a ray of a 2-D Hilbert space, that is as a vector of a 2-D Hilbert spaces apart a constant coefficient).

We can identify the qubits by this vectors:

$$\begin{bmatrix} \cos(\vartheta/2) \\ e^{i\phi} \cdot \sin(\vartheta/2) \end{bmatrix}$$

characterized by two parameters (ϑ, ϕ), that can be seen as the spherical coordinates of a point $P(\vartheta, \phi)$ onto a surface of a sphere of radius 1. This sphere representing qubits is the BLOCH'S SPHERE.



The north-pole is characterized by a co-latitude $\vartheta = 0$, so $\begin{bmatrix} 1 \\ 0 \end{bmatrix} \equiv |0\rangle$

The south-pole is characterized by a co-latitude $\vartheta = \pi$ and $\phi = 0$, so $e^{i\phi} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \equiv e^{i\phi} \cdot |1\rangle = |1\rangle$

$|0\rangle$ and $|1\rangle$ are orthogonal qubits, so they are opposite points on Bloch's sphere.

$|0\rangle$ and $|1\rangle$ are eigenkets of the Z-Pauli operator $(\hat{\sigma}_3)$, so the points on Bloch's sphere are the intersection with z-axis.

We know that the eigenkets of the X-Pauli's operator are $|+\rangle$ and $|-\rangle$ $\Rightarrow$ the representing points are the intersection with the x-axis.

EXERCISE: Verify the intersection $|+i\rangle$

SOLUTION:

$$|+i\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + i|1\rangle\right)$$

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1\\ i\end{bmatrix} \equiv \begin{bmatrix}\cos(\vartheta/2)\\ e^{i\phi}\sin(\vartheta/2)\end{bmatrix}$$

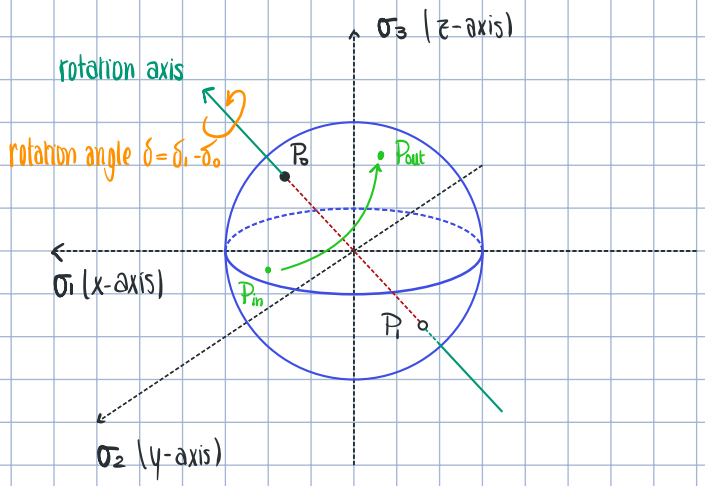
$\cos \vartheta/2 = 1/\sqrt{2} \quad \Rightarrow \quad \vartheta/2 = \pi/4 \quad \Rightarrow \quad \vartheta = \pi/2$

$\sin \vartheta/2 = 1/\sqrt{2}$ for $\vartheta = \pi/2 \quad \Rightarrow \quad e^{i\phi} = i \quad \Rightarrow \quad \phi = \pi/2$

A quantum gate $\hat{U}$ represented by a unitary operator with two orthonormal eigenkets $|\varphi_0\rangle$, $|\varphi_1\rangle$ and corrisponding eigenvalues $e^{i\phi_0}$, $e^{i\phi_1}$ (respectively) and expressed by the spectral decomposition:

$$\hat{U} = e^{i\delta_0}\,\hat{\Pi}_{|\varphi_0\rangle} + e^{i\delta_1}\,\hat{\Pi}_{|\varphi_1\rangle}$$

can be described by a rotation on the Bloch's sphere around an axis passing through the center of the sphere and joining the points of the eigenkets, with rotation angle $\delta = \delta_1 - \delta_0$ (phase difference between eigenvalues).



$|\varphi_0\rangle \longleftrightarrow P_0$

$|\varphi_1\rangle \longleftrightarrow P_1$

P_0, P_1 are diametrically opposite

Positive δ means anticlockwise rotation

$$|\psi_{out}\rangle = \hat{U}\,|\psi_{in}\rangle \xrightarrow{\text{Bloch's sphere representation}} P_{in} \xrightarrow{\text{rotation due to the action of } \hat{U}} P_{out}$$

If φ is an eigenket of $\hat{U}$, then $\hat{U}\,|\varphi_{0,1}\rangle = e^{i\delta_{0,1}}\,|\varphi_{0,1}\rangle$

same qubit means same point on the Bloch's sphere

The X-Pauli's operator

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \text{(quantum not)}$$

with eigenkets $|+\rangle$ and $|-\rangle$ and eigenvalues $+1$ and -1 (respectively)

$$\begin{cases} e^{i\delta_0} = 1 \longrightarrow \delta_0 = 0 \\ e^{i\delta_1} = -1 \longrightarrow \delta_1 = \pi \end{cases}$$

$$\delta = \delta_1 - \delta_0 = \pi$$

binary rotation

We have a rotation of π (anti-clockwise) around the rotation axis $\overrightarrow{P_1P_0}$

x axis (that's why it is named "X-Pauli operators")

$\hat{X}^2 = \hat{X}\cdot\hat{X} = \hat{1}$ → two consecutive rotations of π around the rotation axis ⇒ identity.

- X - Pauli's operator $\longleftrightarrow$ binary rotation around the x-axis
- Y - Pauli's operator $\longleftrightarrow$ binary rotation around the y-axis
- Z - Pauli's operator $\longleftrightarrow$ binary rotation around the z-axis

For example:

$$|+\rangle \longrightarrow \boxed{\hat{Z}} \longrightarrow \hat{Z}|+\rangle = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \longleftrightarrow |-\rangle$$

As seen on the Bloch's sphere

In general, a Pauli's operator is:

$\hat{\sigma}_{\vec{u}} = u_x \cdot \hat{X} + u_y \cdot \hat{Y} + u_z \cdot \hat{Z}$ where $\vec{u} = (u_x, u_y, u_z)$ is a Bloch's vector (unitary-length vector)

Example:

$X \equiv \sigma_x$ with $\vec{u} = (1, 0, 0)$

↳ $\hat{\sigma}_{\vec{u}}$ is described on Bloch's sphere by a binary rotation around $\vec{u}$.

The eigenket of $\hat{\sigma}_{\vec{u}}$ are represented by the points

$P_0 (u_x, u_y, u_z)$

$P_1 (-u_x, -u_y, -u_z)$

where $\vec{u} = (u_x, u_y, u_z)$

Hadamar gate

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$\hat{H}|0\rangle = |+\rangle$

$\hat{H}|1\rangle = |-\rangle$

Z - basis $\xrightarrow{\hat{H}}$ X - basis

$\{|0\rangle, |1\rangle\}$ is the Z-basis (computational basis)

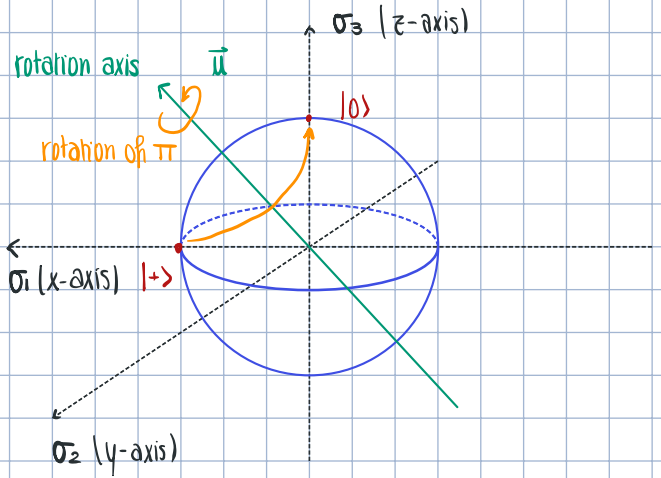
$\{|+\rangle, |-\rangle\}$ is the X-basis

$\{|+i\rangle, |-i\rangle\}$ is the Y-basis

$$\hat{H} = \frac{\hat{X}+\hat{Z}}{\sqrt{2}} = u_x \cdot \hat{X} + u_y \cdot \hat{Y} + u_z \cdot \hat{Z}$$

$u_x = 1/\sqrt{2}$, $u_y = 0$, $u_z = 1/\sqrt{2}$

↳ binary rotation around the axis identified by: $\vec{u} = \frac{1}{\sqrt{2}}(1,0,1) \Rightarrow$ bisectrix of (x,z) plane



$$\hat{H}|+\rangle = |0\rangle$$

$$\hat{H}^{-1} \cdot \hat{H}|+\rangle = \hat{H}^{-1}|0\rangle$$

$$|+\rangle = \hat{H}^{-1}|0\rangle$$

For a Pauli's operator:

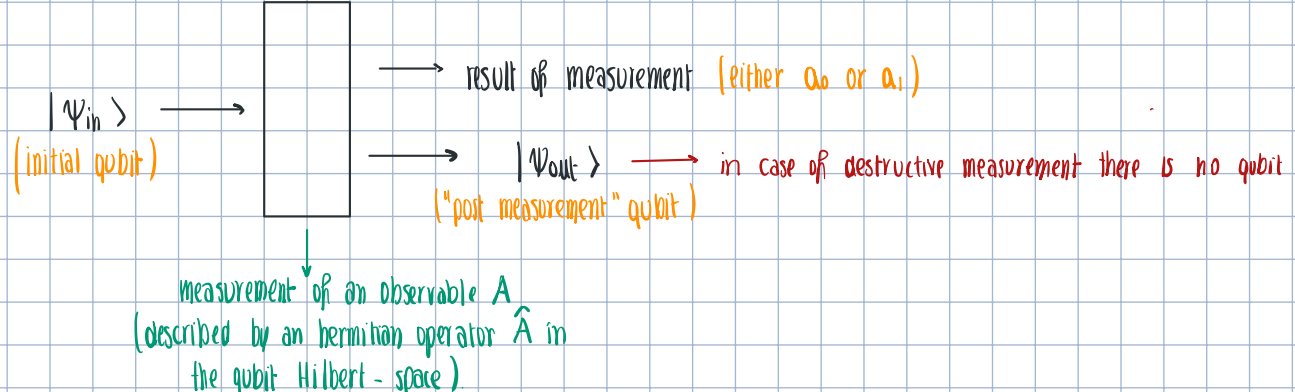
$$\hat{H}^{-1} = \hat{H}^{+} = \hat{H}$$

($\hat{H}^{+}$: hermitian; $\hat{H}^{-1}$: unitary)

$$\hat{H}^{-1}|0\rangle = \hat{H}|0\rangle = |+\rangle$$

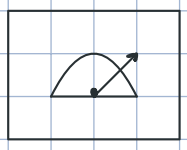
But also: $\hat{H}|1\rangle = |-\rangle$

MEASUREMENT PROCESS ON A QUBIT



where:

$$\begin{cases} \hat{A}|\varphi_0\rangle = a_0|\varphi_0\rangle \\ \hat{A}|\varphi_1\rangle = a_1|\varphi_1\rangle \end{cases}$$



$|\psi_{in}\rangle \longrightarrow$ → measurement result = $\begin{cases} (1) \text{ bit } 0 \\ (-1) \text{ bit } 1 \end{cases}$

→ $|\psi_{out}\rangle = \begin{cases} (|0\rangle) \text{ bit } 0 \\ (|1\rangle) \text{ bit } 1 \end{cases}$

↑ infinite number of possibilities: $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$

↓ measurement of Z observable or measurement in the computational basis (Z-basis)

$\{|0\rangle, |1\rangle\}$ for qubits.

We have a random irreversible process with probabilities:

$$\begin{cases} P_0 \text{ (probability of obtaining bit 0)} = F(\psi_{in}, 0) = |\langle 0|\psi_{in}\rangle|^2 \\ P_1 \text{ (probability of obtaining bit 1)} = F(\psi_{in}, 1) = |\langle 1|\psi_{in}\rangle|^2 \end{cases}$$

considering the orthonormal basis $\{|0\rangle, |1\rangle\}$.

$$P_0 + P_1 = 1$$

We can also write

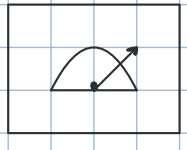
$$\begin{cases} P_0 = \langle \psi_{in} | \hat{\Pi}_{|0\rangle} | \psi_{in} \rangle \\ P_1 = \langle \psi_{in} | \hat{\Pi}_{|1\rangle} | \psi_{in} \rangle \end{cases}$$

$P_0 + P_1 = 1$ because $\hat{\Pi}_{|0\rangle} + \hat{\Pi}_{|1\rangle} = \hat{1}$.

The only case of deterministic measure on a qubit is when the qubit is an eigenstate of the observable (that is the qubit is one of the two basis-states of measurement).

No-cloning theorem: it is not possible to clone an unknown qubit except for the case in which the qubit is one of the two basis states of the measurement.

Example:



$|\psi_{in}\rangle \longrightarrow$ → measurement result (bit 0 or bit 1)

→ if you measure bit 0 then $|\psi_{out}\rangle = |0\rangle$ and $|\psi_{in}\rangle = |0\rangle$

(either $|0\rangle$ or $|1\rangle$)

It is possible to demonstrate that the Pauli's operators $\{\hat{X}, \hat{Y}, \hat{Z}\}$ form a maximal set of complementary observable.

Two observable A, B are said complementary when they are not compatible ($[A,B] \neq 0$) and when the eigenket bases are mutually unbiased:

$\{ |\varphi_0^{(A)}\rangle , |\varphi_1^{(A)}\rangle \}$ A-basis (formed by the eigenkets of A)

$\{ |\varphi_0^{(B)}\rangle , |\varphi_1^{(B)}\rangle \}$ B-basis

$|\langle \varphi_m^{(A)} | \varphi_n^{(B)} \rangle|^2$ = independent from m,n = constant = $\frac{1}{2}$ (for qubits)

($m,n = 0,1$ for qubits)

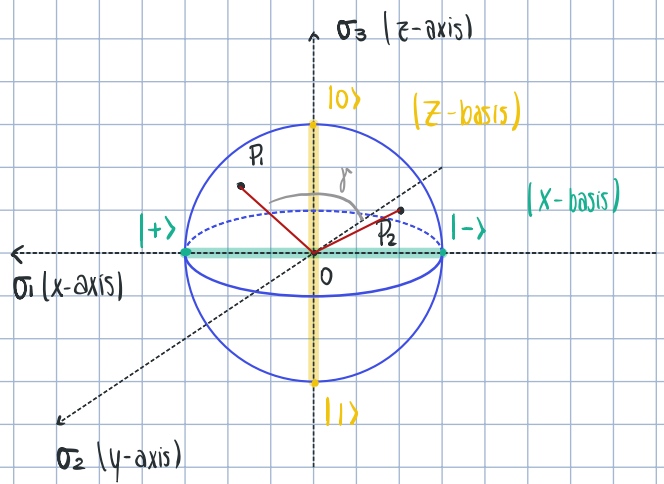
$[X,Y] = 2i \cdot Z$ (we can verify by exercise)

$[Y,Z] = 2i \cdot X$

$[Z,X] = 2i \cdot Y$

Moreover:

$[X,Y] = -[Y,X]$



The fidelity between qubits $|\psi_1\rangle$, $|\psi_2\rangle$ is

$$F(\psi_1,\psi_2) = |\langle \psi_2 | \psi_1 \rangle|^2$$

$$= \cos^2\left(\frac{\widehat{P_1 O P_2}}{2}\right) = \cos^2\left(\frac{\gamma}{2}\right)$$

If $\gamma = \pi$, then P_1 and P_2 are diametrically opposite $\Rightarrow$ fidelity $= \cos^2(\pi/2) = 0$

$\Rightarrow |\langle \psi_2 | \psi_1 \rangle|^2 = 0$

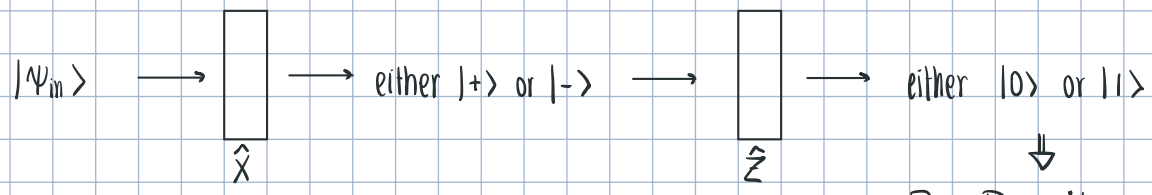
$\langle \psi_2 | \psi_1 \rangle = 0$ (orthogonal states)

$|\langle 0|+\rangle|^2 = \cos^2((\pi/2)/2) = 1/2$

$|\langle 0|-\rangle|^2 = \ldots = 1/2$

$|\langle 1|+\rangle|^2 = \ldots = 1/2$

$|\langle 1|-\rangle|^2 = \ldots = 1/2$



$$P_0 = P_1 = 1/2$$

$$P_0 = \begin{cases} |\langle 0|+\rangle|^2 = 1/2 \\ |\langle 0|-\rangle|^2 = 1/2 \end{cases}$$

$$P_1 = \begin{cases} |\langle 1|+\rangle|^2 = 1/2 \\ |\langle 1|-\rangle|^2 = 1/2 \end{cases}$$