II - THE MATHEMATICAL STRUCTURE OF QUANTUM MECHANICS

1. Review of Basic Concepts

Def.: A complex vector space $\mathcal{H}$ is a non-empty set of elements, called vectors, together with two operations

(A) vector addition

$$+ : \mathcal{H} \times \mathcal{H} \longrightarrow \mathcal{H}$$
$$(u, v) \longmapsto u + v$$

(M) by scalar multiplication

$$\cdot : \mathbb{C} \times \mathcal{H} \longrightarrow \mathcal{H}$$
$$(\lambda, u) \longmapsto \lambda u$$

such that (A) forms an abelian group and (M) satisfies

M1) $(\lambda + \mu) v = \lambda v + \mu v$

M2) $(\lambda \mu) v = \lambda (\mu v)$

M3) $\lambda (u + v) = \lambda u + \lambda v$

M4) $1 v = v$

for all $\lambda, \mu \in \mathbb{C}$ and $u, v \in \mathcal{H}$.

Def.: A inner product space $\mathcal{H}$ is a vector space with an additional map

$$(\, , \,) : \mathcal{H} \times \mathcal{H} \longrightarrow \mathbb{C}$$
$$(u, v) \longmapsto \langle u | v \rangle$$

such that $\forall \; u, v, w \in \mathcal{H}$ and $\lambda, \mu \in \mathbb{C}$ we have

(i) $\langle u, v \rangle = \langle v | u \rangle^*$

(ii) $\langle u | \lambda v + \mu w \rangle = \lambda \langle u | v \rangle + \mu \langle u | w \rangle$

(iii) $\langle u | u \rangle > 0 \Leftarrow u \neq 0$

 Exercise: Show that $\langle u | 0 \rangle = 0 \quad \forall u \in \mathcal{H}$

Note that $\mathcal{H}$ inherits a natural norm from the inner product. In fact we have.

<u>Def.</u>: The <u>norm</u> of a vector in $\mathcal{H}$ is the mapping

$$\| \ \| : \mathcal{H} \longrightarrow \mathbb{R}$$
$$v \longmapsto \|v\| = \langle v | v \rangle^{1/2}$$

In QM the notion of operator as a linear transformation from $\mathcal{H}$ to $\mathcal{H}$ shall play a crucial hole.

<u>Def.</u>: A <u>linear transformation</u> T is a map $T : V \to W$ where V and W are vector spaces over the same field such that

$$T(\lambda u + \mu v) = \lambda T(u) + \mu T(v)$$

for all $u, v \in V$ and $\lambda, \mu \in \mathbb{C}$. We denote the set of all linear transformations from V to W by $L(V, W)$. For the particular case $W = V$, we say that T is a (linear) <u>operator</u> on V and denote $T \in L(V) \equiv L(V, W)$.

2. Basic Concepts in QM

Def.: The physical states in QM are described by non zero vectors in a complex inner product space $\mathcal{H}$. Two vectors describe the same state iff they are multiple of each other.

Examples:

Ex. 1: $\mathcal{H} = L^2(0, a)$

$$\left.\begin{array}{l} \psi : [0,a] \longrightarrow \mathbb{C} \\ \quad x \longmapsto \psi(x) \\ 0 = \psi(0) = \psi(a) \\ \displaystyle\int_0^a |\psi(x)|^2 dx < \infty \end{array}\right\} \psi \in \mathcal{H}$$

inner product: Given $\psi, \phi \in \mathcal{H} = L^2(0,a)$, by definition we have

$$\langle \psi | \phi \rangle \equiv \int_0^a \psi^*(x)\, \phi(x)\, dx$$

Orthonormal basis for $L^2(0,a)$:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad n = 1, 2, 3, \ldots$$

$$\langle \psi_n, \psi_m \rangle = \frac{2}{a} \int_0^a \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx = \delta_{n,m}$$

(See pg 33 of Griffiths)

Given an arbitrary complex function $f \in L^2(0,a)$ we may always write

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin \frac{n\pi x}{a}$$

with

$$c_n = \sqrt{\frac{2}{a}} \int_0^a f(x) \sin \frac{n\pi x}{a}\, dx$$

$$= \int_0^a f(x)\, \psi_n(x)\, dx = \langle \psi_n | f \rangle$$

Ex. 2: $\mathcal{H} = L^2$

$$\left.\begin{array}{l} \psi : \mathbb{R} \longrightarrow \mathbb{C} \\ \quad x \longmapsto \psi(x) \\ \displaystyle\int_{-\infty}^{+\infty} |\psi(x)|^2 dx < \infty \end{array}\right\} \quad \psi \in \mathcal{H} = L^2$$

Given $\phi, \psi \in L^2$, the inner product reads

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

Ex. 3 : Hydrogen-like atom bound state wave functions

$$\left.\begin{array}{l}
\psi : \mathbb{R}^3 \setminus \{0\} \longrightarrow \mathbb{C} \\
\quad (r,\theta,\phi) \longmapsto \psi(r,\theta,\phi) \\
\\
\psi(r,\theta,\phi) = \displaystyle\sum_{n,\ell,m} c_{n\ell m} R_{n\ell}(r)\, Y_\ell^m(\theta,\phi) \\
\\
n = 1, 2, 3, \ldots \\
\ell = 0, 1, 2, \ldots, n-1 \\
m = -\ell, \ldots, -1, 0, \ldots, \ell \\
c_{n\ell m} \in \mathbb{C}
\end{array}\right\} \psi \in \mathcal{H}$$

Given $\psi, \phi \in \mathcal{H}$ the inner product reads

$$\langle \psi | \phi \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \psi^*(r,\theta,\phi)\, \phi(r,\theta,\phi)\, r^2 \sin\theta \, d\phi\, d\theta\, dr$$

Ex. 4 :

$$\left.\begin{array}{l}
\mathcal{H} = \mathbb{C}^2 \\
\\
\psi : \{1,2\} \longrightarrow \mathbb{C} \\
\qquad n \longmapsto \psi_n \\
\\
\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}
\end{array}\right\}$$

$\psi = (\psi_1, \psi_2) \in \mathbb{C}^2$

Orthonormal basis

$e_1 = (1,0), \quad e_2 = (0,1)$

$\psi = (\psi_1, \psi_2) = \psi_1 e_1 + \psi_2 e_2$

or

$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \psi_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Given $\psi, \phi \in \mathcal{H} = \mathbb{C}^2$ we define the inner product

$$\langle \psi | \phi \rangle = (\psi_1^* \quad \psi_2^*) \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$$

$$= \psi_1^* \phi_1 + \psi_2^* \phi_2 \in \mathbb{C}$$

3. Dirac Notation

In Dirac's notation we denote the vector $\psi \in \mathcal{H}$ by $|\psi\rangle$. For instance in the case $\mathcal{H} = \mathbb{C}^2$:

$$\psi = (\psi_1, \psi_2) \in \mathbb{C}^2 \quad \longleftrightarrow \quad |\psi\rangle = (\psi_1, \psi_2) \in \mathbb{C}^2$$

orthonormal basis: $\longleftrightarrow$ $|+\rangle = (1, 0)$

$e_1 = (1, 0)$ $\quad |-\rangle = (0, 1)$

$e_2 = (0, 1)$

$$\psi = (\psi_1, \psi_2) = \psi_1 (1, 0) + \psi_2 (0, 1) \quad \longleftrightarrow \quad |\psi\rangle = \psi_1 |+\rangle + \psi_2 |-\rangle$$

Or else consider the case $\mathcal{H} = L^2$

$\psi \in L^2 \quad \longleftrightarrow \quad |\psi\rangle \in L^2$

$\psi : \mathbb{R} \to \mathbb{C}$

$y \longmapsto \psi(y)$

basis :

$\psi_x(y) = \delta(x-y)$

$$\psi(y) = \int dx \; \delta(x-y)\, \psi(x)$$

$$= \int dx \; \psi(x)\, \delta(x-y)$$

$$= \int dx \; \underbrace{\psi(x)}_{\text{coefficients (or components)}} \psi_x(y)$$

DIRAC NOTATION

basis :

$|x\rangle \to$ particle localized at the point x.

$|\psi\rangle \to$ state described by wave-function $\psi(y)$

$$|\psi\rangle = \int dx \; c(x)\, |x\rangle$$

vector written as linear combination of basis vectors $|x\rangle$.

The coefficients $c(x)$ are

$c(x) = \langle x | \psi \rangle$ ← inner product

$$= \int dy \; \delta(x-y)\, \psi(y)$$

$$= \psi(x)$$

$\therefore \boxed{\psi(x) = \langle x | \psi \rangle \text{ (Dirac notation)}}$

4. Operators in QM

Def.: The <u>observables</u> in QM are described by self-adjoint operators in $\mathcal{H}$.

Def.: The adjoint $A^\dagger$ of an operator $A \in L(\mathcal{H})$ is defined by

$$\langle A^\dagger \phi | \psi \rangle = \langle \phi | A \psi \rangle, \quad \forall \psi, \phi \in \mathcal{H}$$

Examples:

Ex. 1: In the Hilbert space $\mathcal{H} = \mathbb{C}^2$ a general operator can be written by a 2×2 complex matrix wrt the canonical basis.

Given $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ with $a, b, c, d \in \mathbb{C}$, what is the corresponding adjoint operator?

~~We have~~ Given $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ and $\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$ we have

$$A\psi = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} a\psi_1 + b\psi_2 \\ c\psi_1 + d\psi_2 \end{pmatrix}$$

$$\langle \phi | A\psi \rangle = (\phi_1^* \quad \phi_2^*) \begin{pmatrix} a\psi_1 + b\psi_2 \\ c\psi_1 + d\psi_2 \end{pmatrix}$$

$$= a\phi_1^*\psi_1 + b\phi_1^*\psi_2 + c\phi_2^*\psi_1 + d\phi_2^*\psi_2$$

Now let $A^+ = \begin{pmatrix} \bar{a} & \bar{b} \\ \bar{c} & \bar{d} \end{pmatrix}$ where $\bar{a}, \bar{b}, \bar{c}, \bar{d}$ are complex numbers to be determined from a, b, c, d.

We have

$$A^+ \phi = \begin{pmatrix} \bar{a} & \bar{b} \\ \bar{c} & \bar{d} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \begin{pmatrix} \bar{a}\phi_1 + \bar{b}\phi_2 \\ \bar{c}\phi_1 + \bar{d}\phi_2 \end{pmatrix}$$

and

$$\langle A^+\phi | \psi \rangle = \left(\bar{a}^*\phi_1^* + \bar{b}^*\phi_2^* \quad \bar{c}^*\phi_1^* + \bar{d}^*\phi_2^* \right) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

$$= \bar{a}^*\phi_1^*\psi_1 + \bar{b}^*\phi_2^*\psi_1 + \bar{c}^*\phi_1^*\psi_2 + \bar{d}^*\phi_2^*\psi_2$$

From the definition $\langle A^+\phi | \psi \rangle = \langle \phi | A\psi \rangle$ we get

$$0 = (a - \bar{a}^*)\phi_1^*\psi_1 + (b - \bar{c}^*)\phi_1^*\psi_2 + (c - \bar{b}^*)\phi_2^*\psi_1 + (d - \bar{d}^*)\phi_2^*\psi_2$$

Since $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ and $\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$ are arbitrary we get

$$\bar{a} = a^*, \quad \bar{b} = c^*, \quad \bar{c} = b^* \text{ and } \bar{d} = d^*.$$

Thus

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Longrightarrow A^+ = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}$$

Ex. 2: $\mathcal{H} = L^2(0,a)$

Given a differentiable function $\psi : [0,a] \to \mathbb{C}$, $\psi \in L^2(0,a)$ we consider the linear operator

$$D : \mathcal{H} \longrightarrow \mathcal{H}$$
$$\psi \longmapsto \psi'$$

I.e., D is the derivative operator:

$$(D\psi)(x) = \psi'(x)$$

$$D\psi = \frac{d}{dx}\psi$$

Let us compute the adjoint $D^\dagger$ of the operator $D = \frac{d}{dx}$. By definition we must have

$$\langle D^\dagger \phi | \psi \rangle = \langle \phi | D\psi \rangle$$

for arbitrary complex functions $\psi, \phi \in \mathcal{H}$. On the one hand

$$\langle \phi | D\psi \rangle = \int_0^a \phi^*(x) \frac{d\psi(x)}{dx} dx$$

$$= - \int_0^a \frac{d\phi^*}{dx}(x)\, \psi(x)\, dx + \phi^*(x)\psi(x) \Big|_0^a$$

$$\langle \phi | D\psi \rangle = - \int_0^a \frac{d\phi^*}{dx}(x)\, \psi(x)\, dx$$

On the other hand

$$\langle D^\dagger \phi | \psi \rangle = \int_0^a (D^\dagger \phi)^*(x)\, \psi(x)\, dx$$

and we must have

$$\int_0^a \left[D^\dagger \phi^*(x) + \frac{d\phi^*}{dx}(x) \right] \psi(x)\, dx = 0$$

$$\int_0^a \left[D^\dagger \phi(x) + \frac{d\phi}{dx}(x) \right] \psi^*(x)\, dx = 0$$

Since ψ is arbitrary we have

$$D^\dagger \phi(x) = - \frac{d\phi}{dx}(x)$$

and since ϕ is also arbitrary we have

$$\boxed{D^\dagger = - \frac{d}{dx}}$$

 So, we recall

Def.: The <u>observables</u> in QM are described by self-adjoint operators in $\mathcal{H}$.

Def.: An operator $A \in L(\mathcal{H})$ is self-adjoint when it coincides with its adjoint. I.e., when

$$A^{+} = A$$

From the two previous examples we see that $\frac{d}{dx}$ is not self-adjoint and, for $\mathcal{H} = \mathbb{C}^2$, the ~~adjo~~ operator

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in L(\mathbb{C}^2)$$

is self-adjoint if

$$A^{+} = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = A$$

which amounts to the general form

$$A = \begin{pmatrix} x & z+iw \\ z-iw & y \end{pmatrix} \quad \text{with } x, y, z, w \in \mathbb{R}$$

for A selfadjoint.

Two important operators in QM are the position and momentum operators

Def.: Position operator $\vec{X} = \cancel{X}\hat{x} + \cancel{Y}\hat{y} + \cancel{Z}\hat{z}$ in $\mathbb{R}^3$:

$$\begin{cases} (X\psi)(x,y,z) = x\,\psi(x,y,z) \\ (Y\psi)(x,y,z) = y\,\psi(x,y,z) \\ (Z\psi)(x,y,z) = z\,\psi(x,y,z) \end{cases}$$

Momentum $\vec{P} = P_x\hat{x} + P_y\hat{j} + P_z\hat{k}$

$$\begin{cases} (P_x\psi)(x,y,z) = -i\hbar\,\frac{\partial\psi}{\partial x}(x,y,z) \\ (P_y\psi)(x,y,z) = -i\hbar\,\frac{\partial\psi}{\partial y}(x,y,z) \\ (P_z\psi)(x,y,z) = -i\hbar\,\frac{\partial\psi}{\partial z}(x,y,z) \end{cases}$$

By noting that $\hat{x}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z} = \vec{\nabla}$ we may also write

$$\boxed{\vec{P} = -i\hbar\vec{\nabla}}$$

In one dimension this reduces to

$$(X\psi)(x) = x\psi(x) \quad \text{and} \quad (P\psi)(x) = -i\hbar\frac{d\psi}{dx}(x)$$

Note that we clearly have issues of domain here becaus for instance

$$\|P\psi\|^2 = \int_{\mathbb{R}} \left|-i\hbar\frac{d\psi}{dx}\right|^2 dx$$

$$\|X\psi\|^2 = \int_{\mathbb{R}} x^2|\psi(x)|^2\,dx$$

An important observable in QM will be the Hamiltonian operator. This operator, specific for each system, will be responsible for the time evolution.

As a particular example we mention

$$(H\psi)(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x}) + V(\vec{x})\psi(\vec{x})$$

In terms of the previous operators

$$\begin{cases} \vec{X}\,\psi(\vec{x}) = \vec{x}\,\psi(\vec{x}) \\ \vec{P}\,\psi(\vec{x}) = -i\hbar\,\vec{\nabla}\psi(\vec{x}) \end{cases}$$

we may rewrite

$$(H\psi)(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x}) + V(\vec{X})\psi(\vec{x})$$

or simply

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{X})$$

i.e.

$$\boxed{H = \frac{\vec{P}^2}{2m} + V(\vec{X})}$$

In this notation the Schrödinger time-independent wave equation can be written as

$$H\psi = E\psi$$

5- Hilbert Spaces

Def.: A Hilbert space is a complete complex inner product space.

Rem 1: Complete wrt the distance function induced by the inner product.

Rem 2: Recall that an inner product space is automatically a vector or linear space.

Rem 3: Complete means that every Cauchy sequence converges.

Cauchy Sequence

Let $\mathcal{H}$ be a complex inner product space. A sequence $\psi_n \in \mathcal{H}$, $n \in \mathbb{N}$, is said to be Cauchy when $\forall\, \epsilon > 0$, there exists a natural N_ϵ such that

$$n, m > N_\epsilon \implies \| \psi_n - \psi_m \| < \epsilon .$$

We recall further that a sequence $\psi_n \in \mathcal{H}$, $n \in \mathbb{N}$, converges to $\psi \in \mathcal{H}$ when for all $\epsilon > 0$ there exists N_ϵ such that

$$n > N_\epsilon \implies \| \psi_n - \psi \| < \epsilon$$

Counterexample

The rational numbers $\mathbb{Q}$ are not complete.

Take for instance the sequence $x_{n+1} = \frac{x_n}{2} + \frac{1}{x_n}$

or $x_n = \dfrac{f_n}{f_{n-1}} \to \dfrac{1+\sqrt{5}}{2} = \varphi$.

If every Cauchy sequence $\psi_m \in \mathcal{H}$ converges to a vector $\psi \in \mathcal{H}$ then, by definition, $\mathcal{H}$ is a Hilbert space.

Separability: A metric space is separable if it contains a countable dense subset.

We recall that a subset $S \subset \mathcal{H}$ is dense in $\mathcal{H}$ if for any vector $\psi \in \mathcal{H}$ there exists a vector $\phi \in S$ such that

$$\| \phi - \psi \| < \epsilon .$$

It is possible to prove that:

A Hilbert space is separable iff it contains a countable orthonormal basis.

6- Statistical Aspects

Def.: The expectation value of an operator A in a state $\psi \in \mathcal{H}$ is defined as

$$\langle A \rangle_\psi = E_\psi (A) \equiv \frac{\langle \psi | A \psi \rangle}{\| \psi \|^2}$$

(Or in Dirac's notation:

$$\langle A \rangle_\psi = \frac{\langle \psi | A | \psi \rangle}{\langle \psi | \psi \rangle}$$)

Example: $A = V(X)$, $X \to$ position operator, ψ normalized

$$< V(X) > = E_\psi (V(X))$$

$$= \frac{< \psi | V(X) \psi >}{\| \psi \|^2}$$

$$= \int \psi^*(x) V(x) \psi(x) \, dx$$

$$= \int |\psi(x)|^2 V(x) dx = \int \rho(x) V(x) \, dx$$

proposition:

Let $\mathcal{H}$ be a Hilbert space and $\psi \in \mathcal{H}$, $\psi \neq 0$, a state vector. Then we have

(i) $\langle A \rangle_\psi = \langle A \rangle_{\lambda\psi}$, for $\lambda \in \mathbb{C}$, $\lambda \neq 0$.

(ii) $\langle A \rangle_\psi \in \mathbb{R} \Longleftarrow A$ is self-adjoint

(iii) $\langle A \rangle_\psi \geq 0 \Longleftarrow A$ is positive

(iv) $\langle \alpha A + \beta B \rangle_\psi = \alpha \langle A \rangle_\psi + \beta \langle B \rangle_\psi$, $\forall A, B \in L(\mathcal{H})$, $\alpha, \beta \in \mathbb{C}$.

proof:

(i) $$\langle A \rangle_{\lambda\psi} = \frac{\langle \lambda\psi | A(\lambda\psi) \rangle}{\langle \lambda\psi | \lambda\psi \rangle} = \frac{\lambda^* \lambda \langle \psi | A\psi \rangle}{\lambda^* \lambda \langle \psi | \psi \rangle} = \frac{\langle \psi | A\psi \rangle}{\| \psi \|^2} = \langle A \rangle_\psi$$

(ii) If A is self-adjoint, i.e., $A^+ = A$, we have

$$\langle A \rangle_\psi^* = \left[\frac{\langle \psi | A\psi \rangle}{\|\psi\|^2} \right]^* \cancel{= \frac{(\langle \psi | A\psi \rangle)^*}{\|\psi\|^2} \neq \langle \psi | A}$$

$$= \left[\frac{\langle \psi | A^+ \psi \rangle}{\|\psi\|^2} \right]^*$$

$$= \frac{\langle A^+ \psi | \psi \rangle}{\|\psi\|^2} = \frac{\langle \psi | A\psi \rangle}{\|\psi\|^2} = \langle A \rangle_\psi$$

since $\langle A \rangle_\psi$ is a complex number satisfying $\langle A \rangle_\psi^* = \langle A \rangle_\psi$ it must be real.

(iii) If A is a positive operator, by definition, for any $\psi \in \mathcal{H}$ we have $\langle \psi | A\psi \rangle > 0$.

Thus it follows

$$\langle A \rangle_\psi = \frac{\langle \psi | A\psi \rangle}{\|\psi\|^2} > 0$$

(iv) $$\langle \alpha A + \beta B \rangle_\psi = \langle \psi | (\alpha A + \beta B)\psi \rangle$$

$$= \langle \psi | \alpha(A\psi) \rangle + \langle \psi | \beta(B\psi) \rangle$$

$$= \alpha \langle \psi | A\psi \rangle + \beta \langle \psi | B\psi \rangle$$

$$= \alpha \langle A \rangle_\psi + \beta \langle B \rangle_\psi$$

The variance of an observable A in the state ψ can be computed as

$$\langle (A - \langle A\rangle_\psi)^2 \rangle_\psi =$$

$$= \langle A^2 - 2A\langle A\rangle_\psi + \langle A\rangle_\psi^2 \rangle_\psi$$

$$= \langle A^2\rangle_\psi - 2\langle A\rangle_\psi \langle A\rangle_\psi + \langle A\rangle_\psi^2$$

$$= \langle A^2\rangle_\psi - \langle A\rangle_\psi^2$$

Def.: The dispersion of the observable A in the state ψ is given by

$$\Delta_\psi(A) = \left(\langle A^2\rangle_\psi - \langle A\rangle_\psi^2 \right)^{1/2}$$

Proposition: The dispersion of A in the state ψ vanishes iff ψ is an A eigenvector. In this last case, the associate eigenvalue is $\langle A\rangle_\psi$.

Proof: First assume that ψ is an A eigenvector, i.e.,

$$A\psi = \lambda\psi$$

Then it immediately follows that

$$\langle A\rangle_\psi = \frac{\langle \psi | A\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\langle\psi|\lambda\psi\rangle}{\langle\psi|\psi\rangle} = \lambda\frac{\langle\psi|\psi\rangle}{\langle\psi|\psi\rangle} = \lambda$$

and

$$\langle A^2\rangle_\psi - \langle A\rangle_\psi^2 = \frac{\langle\psi|A^2\psi\rangle}{\langle\psi|\psi\rangle} - \lambda^2 = \frac{\lambda^2\langle\psi|\psi\rangle}{\langle\psi|\psi\rangle} - \lambda^2 = 0$$

To prove the converse we must use the fact that A is self-ajoint, i.e., $A^+ = A$. In fact, assume that the dispersion of A in the state ψ vanishes. Then it follows

$$0 = \langle A - \langle A\rangle_\psi \rangle^2 = \langle\psi|\,(A - \langle A\rangle_\psi)(A - \langle A\rangle_\psi)\psi\rangle$$

$$= \langle (A - \langle A\rangle_\psi)^+\psi \,|\, (A - \langle A\rangle_\psi)\psi\rangle$$

$$= \langle \underbrace{(A^+ - \langle A\rangle_\psi^*)}_{= A - \langle A\rangle_\psi \text{ because } A \text{ is self-adjoint}}\psi \,|\, (A - \langle A\rangle_\psi)\psi\rangle$$

$$\therefore \quad 0 = \langle (A - \langle A\rangle_\psi)\psi \,|\, (A - \langle A\rangle_\psi)\psi\rangle$$

$$= \|(A - \langle A\rangle_\psi)\psi\|^2$$

$$\therefore \quad (A - \langle A\rangle_\psi)\psi = 0$$

$$\therefore \quad \boxed{A\psi = \langle A\rangle_\psi\,\psi}$$

q.e.d.

Proposition: The eigenvalues of a self-adjoint operator are real.

proof: We have already shown that if A is self-adjoint then $\langle A \rangle_\psi \in \mathbb{R}$, for any non null $\psi \in \mathcal{H}$. If λ is an A-eigenvalue there exists a non null $\psi \in \mathcal{H}$ such that $A\psi = \lambda\psi$ and $\langle A \rangle_\psi$. Thus $\lambda \in \mathbb{R}$.

Proposition: Two eigenvectors ψ, ϕ of a self-adjoint operator A associated to distinct eigenvalues are orthogonal.

proof: Assume $\lambda \neq \mu$ are two distinct A-eigenvalues & and let $\psi, \phi \neq 0$ be two corresponding eigenvectors, i.e.,

$$\begin{cases} A\psi = \lambda\psi \\ A\phi = \mu\phi \end{cases}$$

Since A is self-adjoint λ and μ are real. Note that

$$\begin{aligned}
0 &= \langle \psi | A\phi \rangle - \langle \psi | A\phi \rangle \\
&= \langle A^\dagger\psi | \phi \rangle - \langle \psi | A\phi \rangle \\
&= \langle A\psi | \phi \rangle - \langle \psi | A\phi \rangle \\
&= \lambda^* \langle \psi | \phi \rangle - \mu \langle \psi | \phi \rangle \\
&= (\lambda^* - \mu) \langle \psi | \phi \rangle = (\lambda - \mu) \langle \psi | \phi \rangle
\end{aligned}$$

From $\lambda \neq \mu$ it follows $\langle \psi | \phi \rangle = 0$.

<u>Example:</u> Considering the one-dimensional square well again, for the m-excited state compute the momentum mean and dispersion.

$$\psi_m(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{m\pi x}{a}\right) \quad , \quad x \in [0,a]$$

$$\langle P \rangle_{\psi_m} = \langle \psi_m | P\psi_m \rangle \qquad P = -i\hbar\frac{d}{dx}$$

$$= -i\hbar \int_0^a \psi_m(x)\,\psi_m'(x)\,dx$$

$$= -\frac{i\hbar}{2}\int_0^a \frac{d}{dx}\left[\psi_m(x)^2\right]dx = 0$$

Actually we see the above results for <u>any</u> state $\psi \in \mathcal{H}$.

Dispersion:

$$[\Delta_\psi(P)]^2 = \langle P^2 \rangle_\psi - \underbrace{\langle P \rangle_\psi^2}_{0}$$

$$= \langle P^2 \rangle_\psi$$

For the m-th excited state: $\qquad H = \frac{P^2}{2m}$

$$[\Delta_{\psi_m}(P)]^2 = \langle \psi_m | P^2 \psi_m \rangle = 2m\langle \psi_m | H\psi_m \rangle$$

$$= 2m E_m = \frac{m^2\pi^2\hbar^2}{a^2}$$

7- Time Evolution

QM Fundamental Postulate (Time Evolution)

Given a Hilbert space $\mathcal{H}$ for a physical QM model there exists a distinguished Hamiltonian operator $H \in T(\mathcal{H})$, self-adjoint, which gives the time evolution of the states as

$$\boxed{i\hbar \frac{d}{dt} \psi_t = H \psi_t}$$

The time evolution of states is then described by

$$\psi_t : \mathbb{R} \longrightarrow \mathcal{H}$$
$$t \longmapsto \psi_t$$

Rem.: We allow for the possibility of $H = H(t)$)

Proposition: When the Hamiltonian commutes with itself for any time we have the solution

$$\psi_t = \exp\left[-\frac{i}{\hbar} \int_0^t H \, dt \right] \psi_0$$

Proof: Computing the time-derivative we have

$$\frac{d}{dt}\left\{ \exp\left[\frac{i}{\hbar}\int_0^t H\,dt\right]\psi_t \right\} = \underbrace{\exp\left[\frac{i}{\hbar}\int_0^t H\,dt\right]\left\{\underbrace{\frac{i}{\hbar}H\psi_t + \frac{d\psi_t}{dt}}_{0}\right\}}_{0}$$

So we have

$$\exp\left[\frac{i}{\hbar}\int_0^t H\,dt\right]\psi_t = C = \text{const}$$

For $t=0$ we have $\psi_t = \psi_0 = C$. Thus

$$\boxed{\psi_t = \exp\left[-\frac{i}{\hbar}\int_0^t H\,dt\right]\psi_0}\,.$$

Def.:

$$U_t \equiv \exp\left[-\frac{i}{\hbar}\int_0^t H\,dt\right]$$

is the <u>time-evolution</u> operator

8. Commutator and Commutation Relations

Motivation: Consider the operators X and P as previously defined and note that for $\psi \in \mathcal{H}$ we have

$$
\begin{aligned}
(PX\psi)(x) &= P(X\psi(x)) \\
&= P(x\psi(x)) \\
&= -i\hbar \frac{d}{dx}(x\psi(x)) = -i\hbar\left[\psi(x) + x\frac{d\psi}{dx}(x)\right] \\
&= -i\hbar\psi(x) - i\hbar x \frac{d\psi}{dx}(x) \\
&= (-i\hbar\psi)(x) - i\hbar X \frac{d\psi}{dx}(x) \\
&= (-i\hbar\psi)(x) + X\Big(\underbrace{-i\hbar\frac{d\psi}{dx}(x)}_{P\psi}\Big) \\
&= -i\hbar\psi(x) + (XP\psi)(x) \\
&= \big((-i\hbar\mathbb{1} + XP)\psi\big)(x)
\end{aligned}
$$

i.e.,

$$\boxed{PX = -i\hbar\mathbb{1} + XP}$$

Definition: Given two operators $A, B \in L(\mathcal{H})$ we define $[A,B] \in L(\mathcal{H})$ as

$$[A,B] = AB - BA$$

Note that

$$[\ ,\ ] : L(\mathcal{H}) \times L(\mathcal{H}) \longrightarrow L(\mathcal{H})$$

We have just shown thus that

$$[P_x, X] = -i\hbar \mathbb{1}$$

Similarly we have

$$[X, P_x] = i\hbar \mathbb{1}$$

$$[X, P_y] = [Y, P_x] = 0 = [X, Y] = [P_x, P_y]$$

or more generally

$$[X_i, P_j] = i\hbar \delta_{ij}$$

Note how the above <u>commutation relations</u> resemble the classical Poisson brackets -

Simmilarly to PB, FJ brackets or DB's, the commutator enjoys the following properties

(i) $[A, B] = -[B, A]$

(ii) $[A, B]$ is linear in both A and B

(iii) $[A, BC] = [A, B]C + B[A, C]$

(iv) $[A, [B, C]] + [[A, B], C] = [B, [A, C]]$

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

Lemma: Let $\mathcal{H}$ be a Hilbert space and $A, B, C \in \mathcal{L}(\mathcal{H})$ self-adjoint operators such that $[A, B] = iC$. Then:

(i) For an arbitrary normalizable $\psi \in \mathcal{H}$ we have

$$\langle A^2\rangle_\psi \langle B^2\rangle_\psi \geq \frac{1}{4} \langle C\rangle_\psi^2 .$$

(ii) Excluding the trivial cases $A = 0$ or $B = 0$ or $\langle A^2\rangle_\psi = \langle B^2\rangle_\psi = 0$, the equality holds iff there exists $\ell \in \mathbb{R}$ such that either

$$(A - i\ell B)\psi = 0 \quad \text{or} \quad (B - i\ell A)\psi = 0$$

Proof: If $A = 0$ or $B = 0$ we have trivially $C = 0$ and

$$0 = \langle A^2\rangle_\psi \langle B^2\rangle_\psi = \frac{1}{4}\langle C^2\rangle_\psi = 0 .$$

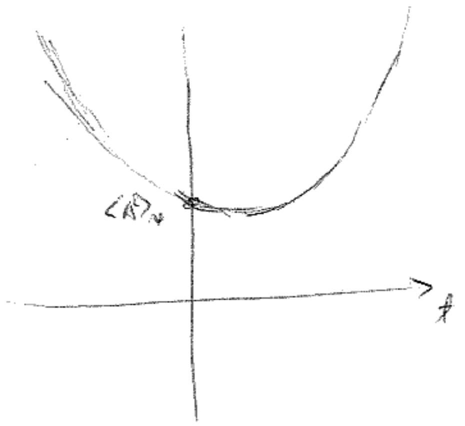
If for a given ψ we have both

$$\langle A^2\rangle_\psi = \langle B^2\rangle_\psi = 0$$

it follows $A\psi = B\psi = 0$ and $\langle C^2\rangle_\psi = 0$ and again we are done.

Thus without loss of generality we assume A and B non null and $\langle B^2\rangle_\psi \neq 0$. Let ℓ denote an arbitrary real variable and construct the following non negative real function

$$\|(A - i\ell B)\psi\|^2 = \langle \psi, (A + i\ell B)(A - i\ell B)\psi\rangle$$
$$= \langle \psi, (A^2 + \ell C + \ell^2 B^2)\psi\rangle$$
$$= \langle B^2\rangle_\psi \ell^2 + \langle C\rangle_\psi \ell + \langle A^2\rangle_\psi \geq 0 .$$



Since the last expression, quadratic in t, is never negative, its discriminant must be non negative

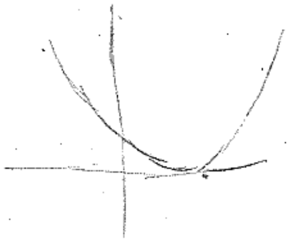
$$\Delta = b^2 - 4ac$$
$$= \langle C \rangle_\psi^2 - 4 \langle A^2 \rangle_\psi \langle B^2 \rangle_\psi \leq 0$$

from which we infer

$$\boxed{\langle A^2 \rangle_\psi \langle B^2 \rangle_\psi \geq \frac{1}{4} \langle C \rangle_\psi^2}$$

The equality holds iff the discriminant is null. In this case

$$\langle A^2 \rangle_\psi \langle B^2 \rangle_\psi = \frac{1}{4} \langle C \rangle_\psi^2$$



and there exists a doubly degenerate solution $t \in \mathbb{R}$ satisfying

$$\| (A - i t B) \psi \|^2 = 0$$

and $(A - i t B)\psi$ must be the null vector:

$$\boxed{(A - i t B) \psi = 0}$$

Remark: In the last expr above $t \in \mathbb{R}$ may be any real number, negative, positive or even zero (of course $t = 0$ means $A\psi = 0$ and $\langle A^2 \rangle_\psi = 0$). We recall we had assumed $\langle B^2 \rangle_\psi = 0$, if that happens to be really the case just switch the roles of A and B to obtain $(B - i t A)\psi = 0$.

Proposition (Heisenberg's Uncertainty Principle)

Let $\mathcal{H}$ denote a Hilbert space and $\psi \in \mathcal{H}$ an arbitrary vector. If $X, P \in L(\mathcal{H})$ satisfy

$$[X, P] = i\hbar$$

then

$$\boxed{\Delta_\psi(X)\, \Delta_\psi(P) \geq \frac{\hbar}{2}}$$

$$\cancel{\langle X\rangle_\psi \langle P\rangle_\psi \geq \frac{\hbar}{2}}$$

Proof: Setting $A = X - \langle X\rangle_\psi$ and $B = P - \langle P\rangle_\psi$ note that

$$[A, B] = [X - \langle X\rangle_\psi, P - \langle P\rangle_\psi]$$
$$= [X, P].$$

Then using

$$\begin{cases} A = X - \langle X\rangle_\psi \\ B = P - \langle P\rangle_\psi \\ C = -i[A, B] = -i\overbrace{[X, P]}^{i\hbar} = \hbar \end{cases}$$

from the previous lemma we get

$$\langle A^2\rangle_\psi \langle B^2\rangle_\psi \geq \frac{1}{4} \langle C\rangle_\psi^2$$

$$\underbrace{\langle (X - \langle X\rangle_\psi)^2\rangle_\psi}_{\Delta_\psi(X)^2} \underbrace{\langle (P - \langle P\rangle_\psi)^2\rangle_\psi}_{\Delta_\psi(P)^2} \geq \frac{1}{4} \underbrace{\langle \hbar\rangle_\psi^2}_{\hbar^2}$$

and taking square roots

$$\boxed{\Delta_\psi(X) \cdot \Delta_\psi(P) \geq \frac{\hbar}{2}}$$

<u>Exercise</u>: Show that in the particular case $\mathcal{H} = L_2$, or similar, $X = x$, $P = -i\hbar \frac{d}{dx}$, the lower bound is achieved iff

$$\psi(x) = c \exp\left\{ -\frac{\ell}{2\hbar} (x-\mu)^2 \right\}$$

for some $\ell \in \mathbb{R}$, $\mu, c \in \mathbb{C}$. To assure normalizability we demand further $\ell > 0$.

<u>Def.</u>: The states ψ for which $\Delta_\psi(X)\Delta_\psi(P) = \frac{\hbar}{2}$ are called minimal uncertainty states.

<u>Example</u>: The ground state for the harmonic oscillator

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$

is a minimal uncertainty state.

Algebraic Solution of the Harmonic Oscillator

Let us consider again the one-dimensional harmonic oscillator.

$$H = \frac{1}{2m} P^2 + \frac{1}{2} m\omega^2 X^2 \qquad P = -i\hbar \frac{d}{dx}$$

$$H\psi = E\psi \qquad P^2 = \hbar^2 \frac{d^2}{dx^2}$$

$$\left(\frac{P^2}{2m} + \frac{1}{2} m\omega^2 X^2 \right) \psi(x) = E\,\psi(x)$$

The Hamiltonian is quadratic in P and X

$$H = \frac{1}{2m} \left(P^2 + m^2\omega^2 X^2 \right)$$

Looking for a factorization of H we define the operators

"The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction." (Sidney Coleman)

$$\begin{cases} a_+ = P + im\omega X \\ a_- = P - im\omega X \end{cases}$$

Recalling that X, P and H are Hermitian, i.e.

$$X^\dagger = X, \quad P^\dagger = P \quad \text{and} \quad H^\dagger = H,$$

we note that

$$\begin{cases} a_+^\dagger = P - im\omega X = a_- \\ a_-^\dagger = P + im X = a_+ \end{cases}$$

That means neither a_+ nor a_- are Hermitian but rather $(a_+^*)^\dagger = a_-$.

A simple operator multiplication shows that

$$a_+ a_- = (P + im\omega X)(P - im\omega X)$$

$$= P^2 + m^2\omega^2 X + im\omega [X, P]$$

$$= 2mH - m\hbar\omega$$

$$a_- a_+ = (P - im\omega X)(P + im\omega X)$$

$$= P^2 + m^2\omega^2 X^2 - im\omega [X, P]$$

$$= 2mH + m\hbar\omega$$

Thus we can factorize H either as

$$\begin{cases} H = \frac{1}{2m}(a_+ a_- + m\hbar\omega) \\ \text{or} \\ H = \frac{1}{2m}(a_- a_+ - m\hbar\omega) \end{cases}$$

Note further that the operators $a_\pm$ enjoy the following simple properties

$$[a_+, a_-] = -2m\hbar\omega, \qquad [a_-, a_+] = 2m\hbar\omega$$

$$[a_+, H] = \frac{1}{2m}[a_+, a_+ a_-] = \frac{a_+}{2m}[a_+, a_-] = -\hbar\omega a_+$$

$$[a_-, H] = \frac{1}{2m}[a_-, a_+ a_-] = \hbar\omega a_-$$

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

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

$$= \langle \psi | a_- a_+ \psi \rangle$$

$$= \langle a_- a_+ \rangle_\psi \|\psi\|^2$$

$$= \langle 2mH + m\hbar\omega \rangle_\psi \|\psi\|^2$$

similarly

$$\|a_-\psi\|^2 = \dots = \langle \psi | a_+ a_- \psi \rangle = \dots = \langle 2mH - m\hbar\omega \rangle_\psi \|\psi\|^2$$

<u>Proposition</u>: Let ψ be an energy eigenvector such that $H\psi = E\psi$. Then

(i) $\|a_\pm \psi\|^2 = 2m\left(E \pm \frac{\hbar\omega}{2}\right)\|\psi\|^2$

(ii) $E \geq \frac{\hbar\omega}{2}$

(iii) $E = \frac{\hbar\omega}{2}$ iff $\psi(x) = \psi_0(x) \equiv A \exp\left[-\frac{m\omega x^2}{2\hbar}\right]$

<u>proof</u>: Recall we had $\|a_\pm\psi\|^2 = 2m\langle H \pm \frac{\hbar\omega}{2}\rangle_\psi \|\psi\|^2$.

For ψ <u>energy eigenvector</u> we have $\langle H \pm \frac{\hbar\omega}{2}\rangle_\psi = E \pm \frac{\hbar\omega}{2}$,

thus in the present case

$$\|a_\pm\psi\|^2 = 2m\left(E \pm \frac{\hbar\omega}{2}\right)\|\psi\|^2$$

(ii) Since $\| a_\pm \psi \|^2 \geq 0$, from

$$\| a_\pm \psi \|^2 = 2m \left(E \pm \frac{\hbar \omega}{2} \right) \| \psi \|^2$$

we get

$$E \pm \frac{\hbar \omega}{2} \geq 0$$

and thus

$$\boxed{E \geq \frac{\hbar \omega}{2}}$$

(iii) From

$$\| a_- \psi \|^2 = 2m \left(E - \frac{\hbar \omega}{2} \right) \| \psi \|^2 \geq 0,$$

the equality holds iff

$$\| a_- \psi \|^2 = 2m \left(E - \frac{\hbar \omega}{2} \right) \| \psi \|^2 = 0$$

i.e.,

$$a_- \psi = 0$$

Using the definition for a_- leads to

$$(P - im\omega X) \psi = 0$$

$$-i\hbar \frac{d\psi}{dx} - im\omega x \psi = 0$$

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

$$\frac{d\psi}{\psi} = -\frac{m\omega x}{\hbar}\, dx$$

$$\ln\left|\frac{\psi(x)}{c}\right| = -\frac{m\omega x^2}{2\hbar}$$

$$\left|\frac{\psi(x)}{c}\right| = \exp\left[-\frac{m\omega x^2}{2\hbar}\right]$$

$$\psi(x) = \pm c \;\exp\left[-\frac{m\omega x^2}{2\hbar}\right]$$

$$\boxed{\psi(x) = A \exp\left[-\frac{m\omega x^2}{2\hbar}\right]}$$

Proposition: Let $H\psi = E\psi$, for $\psi \neq 0$. Then

(i) $H\, a_\pm^n \psi = (E \pm n\hbar\omega)\, a_\pm^n \psi$

(ii) $a_+^n \psi \neq 0$

(iii) $a_-^n \psi = 0 \iff E \in \left\{ \frac{\hbar\omega}{2}, \frac{3\hbar\omega}{2}, \dots, (n-\tfrac{1}{2})\hbar\omega \right\}$

proof: (i) By induction in n: For $n=1$, using

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

we have

$$[H, a_\pm]\psi = \pm\hbar\omega\, a_\pm \psi$$

$$[H, a_\pm]\psi = \pm\hbar\omega a_\pm \psi$$

$$H a_\pm \psi = a_\pm \overbrace{H\psi}^{E\psi} \pm \hbar\omega a_\pm \psi$$

$$H(a_\pm\psi) = (E \pm \hbar\omega)(a_\pm\psi) \longrightarrow \text{true for } n=1 .$$

Next, assuming we have

$$H a_\pm^n \psi = (E \pm n\hbar\omega)\, a_\pm^n \psi$$

it follows that

$$H a_\pm^{n+1}\psi = H a_\pm a_\pm^n \psi$$

$$= \big(\underbrace{[H, a_\pm]}_{\pm\hbar\omega a_\pm} + a_\pm H\big) a_\pm^n \psi$$

$$= \pm\hbar\omega a_\pm^{n+1}\psi + a_\pm (E \pm n\hbar\omega) a_\pm^n \psi$$

$$= \big(E \pm (n+1)\hbar\omega\big) a_\pm^{n+1}\psi$$

(ii) Again we use induction in n. For $n=1$, since $\psi \neq 0$ we have

$$\|a_+\psi\|^2 = \langle \psi | a_- a_+ \psi\rangle = 2m\left(E + \frac{\hbar\omega}{2}\right)\|\psi\|^2$$

As $E \geq \frac{\hbar\omega}{2}$, this cannot vanish and

$$a_+\psi \neq 0$$

Next assume $a_+^m \psi \neq 0$. Then

$$\| a_+^{m+1} \|^2 = \langle a_+^{m+1} \psi | a_+^{m+1} \psi \rangle$$

$$= \langle a_+^m \psi | (a_- a_+) a_+^m \psi \rangle$$

$$= \langle a_+^m \psi | (2mH + m\hbar\omega) a_+^m \psi \rangle$$

$$= 2m \left(E + (m+\tfrac{1}{2}) \hbar\omega \right) \| a_+^m \psi \|^2 \neq 0.$$

(iii) By induction in m. If $m=1$ we already know that

$$a_- \psi = 0 \iff \| a_- \psi \|^2 = 0 \iff 2m\left(E - \frac{\hbar\omega}{2}\right) \|\psi\|^2 = 0.$$

Since $\|\psi\|^2 \neq 0$ we conclude $a_- \psi = 0 \iff E = \frac{\hbar\omega}{2}$.

Next assume the statement is true for some fixed m.

That is, we have:

$H\psi = E\psi$, $\psi \neq 0$ (ψ is an eigenvector with eigenvalue E).

$H(a_-^m \psi) = (E - m\hbar\omega) a_-^m \psi$ ($a_-^m \psi$ is either an eigenvector with eigenvalue $E - m\hbar\omega$ or zero).

Assume $a_-^{m+1} \psi = 0$. Then $a_-^m \psi$ is in the kernel of a_-, which consists of multiples of ψ_0.

Thus either $a_-^m \psi$ is an eigenvector with eigenvalue $\frac{\hbar\omega}{2}$ and we must have $E - m\hbar\omega = \frac{\hbar\omega}{2}$ implying $E = (m+\frac{1}{2})\hbar\omega$ or $a_-^m \psi = 0$ and by the induction hypothesis $E \in \{ \frac{\hbar\omega}{2}, \frac{3}{2}\hbar\omega, \dots, (m-\frac{1}{2})\hbar\omega \}$.

<u>Theorem</u>. The set of eigenvalues of

$$H = \frac{P^2}{2m} + \frac{1}{2} m \omega^2 X^2$$

is

$$\left\{ (n+\tfrac{1}{2}) \hbar\omega, \quad n = 0, 1, 2, \dots \right\}$$

and the corresponding eigenvectors are multiples of

$$\psi_n = a_+^n \psi_0$$

with

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$

<u>Proof</u>: On the one hand, $H\psi_0 = \frac{\hbar\omega}{2}\psi_0$ means precisely that ψ_0 is an eigenvector with minimal eigenvalue $\frac{\hbar\omega}{2}$. We thus have

$$\begin{aligned} H a_+^n \psi_0 &= (E_0 + n\hbar\omega)\, a_+^n \psi_0 \\ &= \left(\frac{\hbar\omega}{2} + n\hbar\omega\right) a_+^n \psi_0 \\ &= (n+\tfrac{1}{2})\hbar\omega\, a_+^n \psi_0 \quad , \quad n = 1, 2, 3, \dots \end{aligned}$$

implying that $\psi_n = a_+^n \psi_0$ are eigenvectors with corresponding eigenvalues $(n+\frac{1}{2})\hbar\omega$. We have thus proved up to now that all $\psi_n = a_+^n \psi_0$ with $n = 0, 1, 2, 3, \dots$ are eigenvectors with eigenvalues $(n+\frac{1}{2})\hbar\omega$, $n = 0, 1, 2, 3, \dots$.

Conversely, assume ψ is an eigenvector with eigenvalue E, i.e., assume

$$H\psi = E\psi \quad \text{with } \psi \neq 0.$$

Choose an arbitrary natural m and aply a_-^m to ψ. The $a_-^m\psi$ is either zero or

$$H\, a_-^m \psi = (E - m\hbar\omega)\, a_-^m \psi$$

If $E - m\hbar\omega < 0$, in the second case we achieve a contradiction with the previous shown fact that all eigenvalues are positive. That means, for a given E, exists $m \in \mathbb{N}$ such that $m > E/\hbar\omega$ and we must have

$$a_-^m \psi = 0$$

leading to

$$E = \left\{ \frac{\hbar\omega}{2}, 3\frac{\hbar\omega}{2}, \dots, (m - \tfrac{1}{2})\hbar\omega \right\}.$$

Finally, to show that the eigenvalues are nondegenerate assume ψ is an eigenvector with eigenvalue $(m+\frac{1}{2})\hbar\omega$. Applying a_- m times we obtain the eigenvalue $\frac{\hbar\omega}{2}$ and we have already shown that the corresponding eigvector is a multiple of ψ_0 I.e.

$$a_-^m \psi = \alpha \psi_0$$

By the same token, starting from ψ_m and applying a_- m times we obtain a multiple of ψ_0:

$$a_-^m \psi_m = \beta \psi_0$$

Note that by hypothesis α and β are non null. That means we have

$$a_-^m \psi = \lambda a_-^m \psi_m .$$

Assume the vector $\psi - \lambda\psi_m$ is non zero. Then it has eigenvalue $(m+\frac{1}{2})\hbar\omega$ and $a_-^m(\psi - \lambda\psi_m) = 0$ gives a contradiction with part (iii) of the previous proposition. Thus we should have

$$\psi = \lambda \psi_m$$

showing the nondegeneracy of level m.