

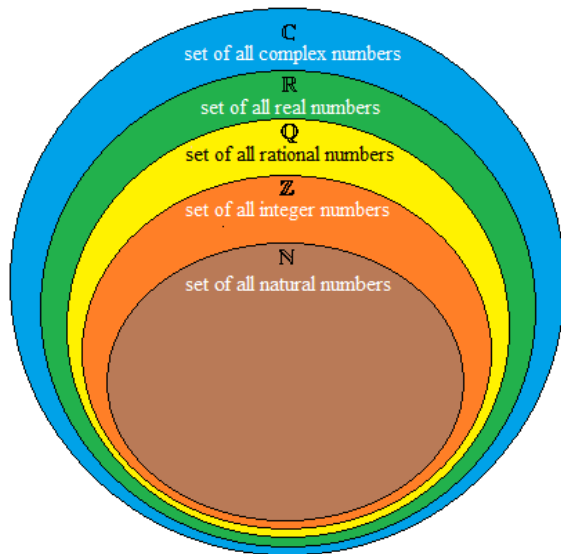
# QUANTUM MECHANICS

## GENERAL FORMALISM FORMULAE

Edited by F. M.

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	(33 Algebra of the two-dimensional harmonic oscillator)	

Numbers set



$\mathbb{N}$  set of all natural numbers

$\mathbb{Z}$  set of all integer numbers

$\mathbb{Z}^+$  set of all positive integer numbers

$\mathbb{Z}^-$  set of all negative integer numbers

$\mathbb{Z}_0^+$  set of all non negative integer numbers

$\mathbb{Z}_0^-$  set of all non positive integer numbers

$\mathbb{Q}$  set of all rational numbers

$\mathbb{R}$  set of all real numbers

$\mathbb{R}^+$  set of all positive real numbers

$\mathbb{R}^-$  set of all negative real numbers

$\mathbb{C}$  set of all complex numbers

$f: M \rightarrow N$  defined by  $x \mapsto f(x)$  application  $f$  of  $M$  in  $N$  defined by  $x$  to which is associated  $f(x)$  ( $f$  maps  $M$  in  $N$ )

$a^*$  indicates the complex conjugated of  $a$

$\Phi(x)$  is the Heaviside step function

$\Delta(x)$  is the Dirac pulse function

$g \circ f$  application's composition ( $g$  composed  $f$ )

**Remark:**

1: Time and position depending vectors, are written in **bold-dark-blue** fonts, while vectors depending only from the position  $r$  are written in **bold-light-blue** fonts.

2: The usual Mathcad complex conjugation operator that is the bar, here means, instead, the arithmetic mean, that is

$$a = \frac{\sum_{j=1}^N a_j}{N}$$

3: the complex conjugation operator is indicated with the asterisk instead of a bar, that is:

if  $z = a + j \cdot b$  then  $z^* = a - j \cdot b$  executable; ( $z^*$  not executable) while "Mathcad" uses a bar:  $\bar{z} = a - j \cdot b$ .

**Unit vectors** in Cartesian coordinates are:  $i_x, i_y, i_z$ .

# 1 Vector spaces

## Cauchy convergence criterion for real sequences.

Given the sequence  $\{a_n\}$ , a necessary and sufficient condition for the convergence of the sequence, is that:

$$\forall \epsilon > 0, \exists N \geq 1 \in \mathbb{Z}: |a_n - a| \leq \epsilon, \forall n \geq N \Rightarrow \lim_{n \rightarrow \infty} a_n = a.$$

Furthermore the criterion say  $\forall \epsilon > 0, \exists N \geq 1 \in \mathbb{Z}: |a_n - a_m| \leq \epsilon, \forall n, m \geq N \Rightarrow \lim_{n \rightarrow \infty} a_n = a.$

## Banach Space (Hyperlink)

A normed and complete space, namely a normed space where every fundamental sequence is convergent, it is a Banach space.

## Hilbert space (Hyperlink)(Hilbert space= $\mathbb{H}$ )

The Cauchy convergence criterion applied to a linear space, is not always sufficient.

When for a linear space, the Cauchy criterion is also sufficient, the space is **complete**.

A complete space, where is also defined the scalar product and consequently the norm, **is a Hilbert space**.

## vector space (Hyperlink)

A vector space  $V$  on a field  $K$  ( $K = \mathbb{R}$  or  $K = \mathbb{C}$ ) is a set where are defined the operations of vector sum

$$(+): V + V \mapsto V \quad (A \mapsto B: \text{read } A \text{ associated } B)$$

$$(v_1, v_2) \rightarrow v_1 + v_2,$$

and the operation of product between a vector and a scalar

$$(\cdot): K \times V \mapsto V$$

$$(\lambda, v) \rightarrow \lambda v$$

▢ Vector spaces Introduction

▢ Examples

▢ Tensors' Theory

## Ket's and bra's algebra

The physical state of an object (for example the orientation of the spin of an atom) is represented by a state's vector in a complex vector space. Following Dirac those vectors belong to a linear or vector space (Set of vectors)

(Hilbert space=  $\mathbb{H}$ ). The vector is indicated by the symbol  $|x\rangle$  (ket) while the linear vector space with  $L = \{|x\rangle\} \in \mathbb{H}$ .

Any linear function  $f$  of the ket  $|\psi\rangle$ , possesses the superposition property, namely:

$$f(\lambda_1 |\psi_1\rangle + \lambda_2 |\psi_2\rangle) = \lambda_1 \cdot f(|\psi_1\rangle) + \lambda_2 \cdot f(|\psi_2\rangle).$$

If two functions  $f_1$  and  $f_2$  have this property (superposition), any linear combination of this two functions:

$$c_1 \cdot f_1 + c_2 \cdot f_2,$$

also has this property. The function  $f(|x\rangle)$  defines the new vector (bra)  $\langle x|$ . The value taken by this function for the ket

$|\psi\rangle$  is the number  $\langle x|\psi\rangle$ .

To the dual space of  $L$  belongs the vector bra  $\langle x|$ , dual of the ket  $|x\rangle$ . There is a one-to-one correspondence between the vectors of the space  $L$  and the vectors of the dual one. The correspondence between each ket and each bra is indicated as a conjugation, namely the bra conjugate to the ket  $|x\rangle$  is represented by  $\langle x|$ . The correspondence is anti linear, that is to the linear combination  $\lambda_2 |x\rangle + \lambda_1 |y\rangle = |z\rangle$  corresponds the bra conjugate

$$\langle z| = \lambda_2^* \langle x| + \lambda_1^* \langle y|.$$

To the ket  $|0\rangle$  corresponds the bra  $\langle 0|$  and vice versa. For the linearity, are necessary two operations: the sum

$|x\rangle + |y\rangle = |z\rangle$  and the product between a complex constant  $\alpha \in \mathbb{C}$ , and the ket  $|x\rangle$ , namely

$$|z\rangle = \alpha |x\rangle = |x\rangle \alpha. \tag{1.1}$$

### Ket vector's properties

$$\exists \text{ Opposite} \quad -|x\rangle + |x\rangle = |0\rangle \tag{1.2}$$

$$\exists \text{ Neutral element (sum)} \quad |0\rangle \text{ namely } |0\rangle + |x\rangle = |x\rangle \tag{1.3}$$

$$\text{Commutative (sum)} \quad |x\rangle + |y\rangle = |y\rangle + |x\rangle \tag{1.4}$$

$$\text{Associative (sum)} \quad (|x\rangle + |y\rangle) + |z\rangle = |x\rangle + (|y\rangle + |z\rangle) \tag{1.5}$$

$$\text{Distributive (sum)} \quad \alpha \cdot (|x\rangle + |y\rangle) = \alpha |x\rangle + \alpha |y\rangle \tag{1.6}$$

$$\text{Distributive (product)} \quad (\alpha + \beta) |x\rangle = \alpha |x\rangle + \beta |x\rangle \tag{1.7}$$

$$\text{Associative (product)} \quad \alpha \cdot (\beta |x\rangle) = (\alpha \cdot \beta) |x\rangle \tag{1.8}$$

$$\text{Identity} \quad 1 |x\rangle = |x\rangle \tag{1.9}$$

$$\text{To the ket } |w\rangle = \int_{\xi_1}^{\xi_2} \lambda(\xi) |\xi\rangle d\xi \text{ corresponds the bra conjugated } \langle w| = \int_{\xi_1}^{\xi_2} \lambda(\xi)^* \langle \xi| d\xi$$

The set  $L = \{|x\rangle\}$  and the two operation  $(+, \cdot)$  verifying the previous axioms, forms a *linear space or vector space*.

Examples of linear sets: a) the set of the complex numbers  $(\cdot, +, -, /)$ ,

b) two and three-dimensional geometric spaces  $(\cdot, +, -, /)$ ,

c) the set  $\text{Mat}$  of the square matrices  $(N \times N)$   $(\cdot, +, -, \text{inverse})$ ,

d) the set of all continuous functions defined on a continuous and established range  $(\cdot, +, -, /)$ .

e) the set of all integrable functions  $(\cdot, +, -, /)$ ,

f) the set of all square integrable functions  $(\cdot, +, -, /)$ ,

g) the set of all function families of functions  $(\cdot, +, -, /)$ .

▢

## 2 Scalar product axioms [4]

Scalar product (or internal product) of two ket vectors ( $|x\rangle, |y\rangle$ ) belonging to the Euclidean and vector space

$L = \{|x\rangle\}$ . The scalar product must associate to each couple of vectors ( $|x\rangle, |y\rangle$ ) a complex number, namely:

$$(|x\rangle, |y\rangle) \rightarrow \alpha = \langle x | y \rangle$$

$$\langle x | y \rangle = \langle x | \cdot | y \rangle \quad (2.1)$$

$$\langle x | x \rangle \geq 0 \quad (2.2)$$

$$\langle x | x \rangle = 0 \Rightarrow |x\rangle = |0\rangle \quad (2.3)$$

$$\langle x | y \rangle = \langle y | x \rangle^* \quad (2.4)$$

$$\langle x | (\alpha \cdot y) \rangle = \alpha \langle x | y \rangle \quad (2.5)$$

$$\langle (\alpha \cdot x) | y \rangle = \alpha^* \langle x | y \rangle \quad (2.6)$$

$$\langle x | (y + z) \rangle = \langle x | y \rangle + \langle x | z \rangle \quad (2.7)$$

$$\text{Norm} \quad \| |x\rangle \| = \sqrt{\langle x | x \rangle} \quad 0 \leq \| |x\rangle \| \leq \infty \quad (2.8)$$

$$\| \alpha |x\rangle \| = (|\alpha|) \| |x\rangle \| \quad (2.9)$$

$$\text{Triangular inequality} \quad \| |x\rangle + |y\rangle \| \leq \| |x\rangle \| + \| |y\rangle \| \quad (2.10)$$

$$\text{Distance} \quad d_{xy} = \| |x\rangle - |y\rangle \| \quad (2.11)$$

External product between a ket  $|x\rangle$  and a bra  $\langle x|$  is the operator:  $|x\rangle \langle x|$ .

(2.12)

## 3 vector analysis

Consider the sequence of vectors  $\{|x_n\rangle\}$ , I define the limit of the sequence as:

$$\lim_{n \rightarrow \infty} |x_n\rangle = |x\rangle \Leftrightarrow \lim_{n \rightarrow \infty} \| |x_n\rangle - |x\rangle \| = 0.$$

(3.1)

Definition of the limit about the vector space ( $L = \{|x(t)\rangle\} \in \mathbb{H}, t \in \mathbb{R}$ ). The function maps  $\mathbb{R}$  on  $L$ , it associates to every  $t$  the ket  $|x(t)\rangle$ .

$$\lim_{t \rightarrow t_0} |x(t)\rangle = |x(t_0)\rangle$$

(3.2)

The property of uniqueness of the limit and all other, derive from the three properties of the norm.

Continuity of the function: when the previous limit exists, the function is continuous. The ket writing, can be symbolically simplified:  $|x(t)\rangle = |t\rangle, |x_1\rangle = |1\rangle, \dots$ . So, I can write:

$$\lim_{t \rightarrow t_0} |t\rangle = |t_0\rangle, \forall \varepsilon > 0, \exists \delta_\varepsilon > 0 : |t - t_0| < \delta \Rightarrow \left| |t\rangle - |t_0\rangle \right| < \varepsilon.$$

(3.3)

Derivative

$$\frac{d}{dt} |t\rangle = \lim_{t \rightarrow t_0} \frac{|t\rangle - |t_0\rangle}{t - t_0}, \text{ etc.}$$

(3.4)

Integration in (a,b):

Integration in (a,b):

$$\text{consider the function: } \sum_{k=1}^n [(t_k - t_{k-1}) |t_k\rangle], t_0 = a, t_n = b,$$

(3.5)

$$\text{if exists the limit: } \lim_{|\delta_k| \rightarrow 0} \sum_{k=1}^n [(t_k - t_{k-1}) |t_k\rangle] = \int |t\rangle dt = |Q\rangle$$

(3.6)

then  $|Q\rangle$  is the integral of  $|t\rangle$ .

$$\text{In (a,b):} \quad |Q(b)\rangle - |Q(a)\rangle = \int_a^b |t\rangle dt. \quad (3.7)$$

Derivative and integral are linear operators.

#### 4 Orthogonal systems of vectors

Consider the set of vectors  $(L = \{ |x_\alpha\rangle \}) \in \mathbb{H}$ ,  $\alpha \in \mathbb{R}$ , it is an orthonormal set of vectors when:

$$\forall \alpha, \beta \in (\mathbb{R}^2), \langle x_\alpha | x_\beta \rangle = \delta_{\alpha\beta} = \begin{cases} 0 & \text{for } (\alpha \neq \beta) \\ 1 & \text{for } (\alpha = \beta) \end{cases}$$

(4.1)

I can demonstrate that necessarily this set is a linearly independent set of vectors.

**A set of orthonormal vectors is also a set of linearly independent vectors.**

**Then the orthonormal system is complete.** In such case it is worth the following vector decomposition:

$$\text{Decomposition: } \forall |x\rangle \quad \forall |x_\alpha\rangle \neq 0 \in L \quad |x\rangle = \sum_{\alpha} \langle x_\alpha | x \rangle |x_\alpha\rangle \quad (4.2)$$

Each ket is, thus, expressible as a linear combination of its components and hence the vector system:

$$(L = \{ |x(t)\rangle \}) \in \mathbb{H},$$

is a complete basis.

Hilbert spaces for which orthonormal and complete vector spaces are at most numerable, are **separable**.

$$\forall |x\rangle, \quad \forall |x_j\rangle \neq 0 \in L = \{ |x(t)\rangle \} \in \mathbb{H} \Rightarrow |x\rangle = \sum_{j=0}^N \langle x_j | x \rangle |x_j\rangle.$$

(4.3)

$$|x\rangle = |x_s\rangle + |x_n\rangle \quad (4.4)$$

$$\langle x_s | x_s \rangle^2 + \langle x_n | x_n \rangle^2 \leq (|\langle x | x \rangle|)^2$$

$$\langle x_s | x_n \rangle = 0 \quad (4.5)$$

Related to the properties of the Hilbert space, follow some examples.

H1) Consider the two complex numbers sequences  $\{a_n\}$  and  $\{b_n\}$  such that:

$$\sum_{n=1}^{\infty} (|a_n|)^2 < \infty, \text{ and } \sum_{n=1}^{\infty} (|b_n|)^2 < \infty.$$

Define the kets  $|a\rangle = \{a_n\}$  and  $|b\rangle = \{b_n\}$ , so that:

$$\langle a | b \rangle = \sum_{n=1}^{\infty} (a_n^* \cdot b_n), \quad (4.6)$$

$$\langle a | (\alpha \cdot b) \rangle = \sum_{n=1}^{\infty} (a_n^* \cdot \alpha \cdot b_n) = \alpha \cdot \sum_{n=1}^{\infty} (a_n^* \cdot b_n), \quad (4.7)$$

$$\langle (\alpha \cdot a) | b \rangle = \sum_{n=1}^{\infty} [(\alpha \cdot a_n)^* \cdot b_n] = \alpha^* \cdot \sum_{n=1}^{\infty} (a_n^* \cdot b_n), \quad (4.8)$$

$$\text{Cauchy criterion: } \forall \epsilon > 0, \exists N \geq 1 \in \mathbb{Z}: |a_n - a| \leq \epsilon, \forall n \geq N \Rightarrow \lim_{n \rightarrow \infty} a_n = a. \quad (4.9)$$

$$\text{Furthermore } \forall \epsilon > 0, \exists N \geq 1 \in \mathbb{Z}: |a_n - a_m| \leq \epsilon, \forall n, m \geq N \Rightarrow \lim_{n \rightarrow \infty} a_n = a.$$

$$\forall \epsilon > 0, \exists N \geq 1 \in \mathbb{Z}: |b_n - b| \leq \epsilon, \forall n \geq N \Rightarrow \lim_{n \rightarrow \infty} b_n = b.$$

$$\forall \epsilon > 0, \exists N \geq 1 \in \mathbb{Z}: |b_n - b_m| \leq \epsilon, \forall n, m \geq N \Rightarrow \lim_{n \rightarrow \infty} b_n = b.$$

So that the space is complete, and therefore it is a Hilbert space.

**Example 1:**

$$|a\rangle = \{1, 2, 3, 4\} \quad |b\rangle = \{5, 6, 7, 8\}$$

$$\langle a | b \rangle = 1 \cdot 5 + 2 \cdot 6 + 3 \cdot 7 + 4 \cdot 8 = 70$$

**Example 2:**

$$a_n := \frac{2^n}{n!} \quad b_n := (-1)^n \cdot \frac{1}{1+n}$$

$$\langle a | b \rangle = \sum_{n=1}^{\infty} \left[ \left( \frac{2^n}{n!} \right)^* \cdot \left[ (-1)^n \cdot \frac{1}{1+n} \right] \right] = \frac{e^{-2}}{2} - \frac{3}{2}$$

**Example 3:**

$$|a\rangle = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \quad |b\rangle = \begin{pmatrix} 5 \\ 6 \\ 7 \\ 8 \end{pmatrix} \quad \langle a | = (1 \ 2 \ 3 \ 4)$$

$$\langle a | b \rangle = (1 \ 2 \ 3 \ 4) \cdot \begin{pmatrix} 5 \\ 6 \\ 7 \\ 8 \end{pmatrix} = 70$$

**Example 4:**

$$|a\rangle = \begin{pmatrix} 1+j \\ 2+j\sqrt{2} \\ 3+j\cdot 4 \\ 4+j\cdot 5 \end{pmatrix} \quad |b\rangle = \begin{pmatrix} 5-j \\ 6+j \\ 7+j\sqrt{3} \\ 8-j\cdot 3 \end{pmatrix}$$

$$\langle a | = (1-j \ 2-j\sqrt{2} \ 3-j\cdot 4 \ 4-j\cdot 5)$$

$$\langle a | b \rangle = (1-j \ 2-j\sqrt{2} \ 3-j\cdot 4 \ 4-j\cdot 5) \cdot \begin{pmatrix} 5-j \\ 6+j \\ 7+j\sqrt{3} \\ 8-j\cdot 3 \end{pmatrix} = 62.342 - 87.289i$$

**Example 5:**

$$|a\rangle = \begin{pmatrix} 1+j \\ 2+j\sqrt{2} \\ 3+j\cdot 4 \\ 4+j\cdot 5 \end{pmatrix} \quad |b\rangle = \begin{pmatrix} 5-j \\ 6+j \\ 7+j\sqrt{3} \\ 8-j\cdot 3 \end{pmatrix}$$

$$\langle b| = (5+j \quad 6-j \quad 7-j\sqrt{3} \quad 8+j\cdot 3)$$

$$Q = |a\rangle \langle b| = \begin{pmatrix} 1+j \\ 2+j\sqrt{2} \\ 3+j\cdot 4 \\ 4+j\cdot 5 \end{pmatrix} \cdot (5+j \quad 6-j \quad 7-j\sqrt{3} \quad 8+j\cdot 3)$$

$$Q = \begin{pmatrix} 4+6i & 7+5i & 8.732+5.268i & 5+11i \\ 8.586+9.071i & 13.414+6.485i & 16.449+6.435i & 11.757+17.314i \\ 11+23i & 22+21i & 27.928+22.804i & 12+41i \\ 15+29i & 29+26i & 36.66+28.072i & 17+52i \end{pmatrix}$$

□

H2) Continue functions space, defined in the range (0,1). Let's consider the two continue functionals f and g, and calculate the scalar product:

$$\langle f | g \rangle = \int_0^1 f(x) \cdot g(x) dx, \quad (4.10)$$

which always exists, been f and g continue functions.

Now see if they satisfy the scalar product axioms:

$$\langle f | \alpha g \rangle = \int_0^1 f(x) \cdot \alpha \cdot g(x) dx = \alpha \cdot \int_0^1 f(x) \cdot g(x) dx = \alpha \langle f(x) | g(x) \rangle, \quad (4.11)$$

$$\langle \alpha f | g \rangle = \int_0^1 (\alpha \cdot f(x)) \cdot g(x) dx = \alpha \cdot \int_0^1 f(x) \cdot g(x) dx = \alpha \langle f(x) | g(x) \rangle, \quad (4.12)$$

$$\langle f | f \rangle \geq 0,$$

(4.13)

and so on.

If the Cauchy's convergence criterion (4.9) is verified, then this vector space is complete and, therefore the continue

$$\text{Cauchy criterion: } \forall \varepsilon > 0, \exists N \geq 1 \in \mathbb{Z}: |a_n - a| \leq \varepsilon, \forall n \geq N \Rightarrow \lim_{n \rightarrow \infty} a_n = a. \quad (4.9)$$

$$\text{Furthermore } \forall \varepsilon > 0, \exists N \geq 1 \in \mathbb{Z}: |a_n - a_m| \leq \varepsilon, \forall n, m \geq N \Rightarrow \lim_{n \rightarrow \infty} a_n = a$$

H3) The spaces  $L^2[a, b]$  (also indicated  $L_2[a, b]$ ) of the (L=Lebesgue) integrable functions is a Hilbert space.

$L^2[0, 2\pi] \supset \left\{ \frac{e^{i \cdot n \cdot x}}{\sqrt{2 \cdot \pi}} \right\}$  is a complete space (convergent sequence) and therefore it is a Hilbert space.

$L^2[-1, 1] \supset \{P(\lambda, \xi)\}$  set of all **Legendre** polynomials, is a complete space and therefore it is a Hilbert space.

$$P(n, x) = \frac{1}{2^n \cdot n!} \cdot \frac{\partial^n}{\partial x^n} (x^2 - 1)^n, \quad f(n, x) = \sqrt{n + \frac{1}{2}} \cdot P(n, x). \quad (4.14)$$

$L^2[-\infty, \infty] \supset \left\{ \int_{-\infty}^{\infty} f(x)^2 dx \right\}$  set of all square summable functions, (**Hermite** polynomials) is a complete space and therefore it is a Hilbert space.

$$H(n, z) = \frac{e^{-z^2}}{\sqrt{2^n \cdot n! \cdot \pi}} \cdot \frac{\partial^n}{\partial z^n} e^{-z^2} = (-1)^n \cdot \frac{2 \cdot n!}{n!} \cdot F\left(-n, \frac{1}{2}, z^2\right). \quad (4.15)$$

## 5 Linear operators [9]



The operator  $\mathbf{A}$  acts on a ket by left:  $\mathbf{A} | y \rangle = | z \rangle$  (5.1)

and on a bra on the right:  $\langle x | \mathbf{A} = \langle y |$  (5.2)

The eigenvalues spectrum of the operator  $\mathbf{A}$ , consists of:

a) a discrete part, i. e. a finite or infinite set of values  $\lambda_n$  with  $n$  integer;

b) a continuous part i. e. a set of values  $\lambda(\nu)$  which is a continuous and monotone function of  $\nu$ .

Properties of the continuous spectrum:

1)  $\lambda(\nu) \in \mathbb{R}$ ,

2) orthonormality of the eigenvectors belonging to distinct eigenvalues:  $\langle y(\nu, r) | y(\nu_1, r_1) \rangle = \Delta(\nu, \nu_1) \cdot \Delta(r, r_1)$

A linear application  $\mathbf{A}: \mathbb{H}_1 \rightarrow \mathbb{H}_2$  ( $\mathbf{A}$  maps  $\mathbb{H}_1$  on  $\mathbb{H}_2$ ), with  $(\mathbb{H}_1, \mathbb{H}_2) \in \mathbb{H}$ , Hilbert space, is a linear operator.

The linear operator  $\mathbf{A}$  is limited if  $\exists c \in \mathbb{C}: \|\mathbf{A} | x \rangle\| \leq |c| \cdot (\| | x \rangle \|), \forall | x \rangle \in \mathbb{H}_1$ .

The set of all limited and linear operators, together the usual composition laws, is indicated with  $[\mathbb{H}_1, \mathbb{H}_2]$ .

$[\mathbb{H}_1, \mathbb{H}_2]$  is a vector space on  $K$  ( $K \in \mathbb{R}$  or  $K \in \mathbb{C}$ ). For each operator  $\mathbf{A}$ , exists a norm  $\|\mathbf{A}\|$ .  $\mathbb{H}_1$  is the domain and

$\mathbb{H}_2$  is the codomium or the operator's *range*  $\mathbf{R}(\mathbf{A})$ .

If  $f_1 \in \mathbb{H}_1$  and  $f_2 \in \mathbb{H}_2$ , the operator  $\mathbf{A}$  lets associate to  $f_1$  the function  $f_2$ , that is:

$$\forall | x \rangle \in D_{\mathbf{A}} \subset \mathbb{H}_1 \Rightarrow \mathbf{A} | x \rangle \in \mathbf{R}(\mathbf{A}) \subset \mathbb{H}_2.$$

Be  $\mathbb{H}_1$  a linear subset of  $\mathbb{H}_2$ , then:

$$\mathbf{A}(\alpha + \beta) = \alpha \cdot \mathbf{A} + \beta \cdot \mathbf{A}, \quad \forall (\alpha, \beta) \in \mathbb{R} \vee \mathbb{C}, \quad \mathbf{A} \in \mathbb{H}, \quad (5.3)$$

$$(\mathbf{A} \cdot \mathbf{B}) | x \rangle = \mathbf{A} \cdot (\mathbf{B} | x \rangle), \quad (5.4)$$

$$\mathbf{A} \cdot (\mathbf{B} \cdot \mathbf{C}) = (\mathbf{A} \cdot \mathbf{B}) \cdot \mathbf{C}, \quad (5.5)$$

$$\mathbf{A} \cdot (\mathbf{B} + \mathbf{C}) = \mathbf{A} \cdot \mathbf{B} + \mathbf{A} \cdot \mathbf{C}, \quad (5.6)$$

$$\mathbf{A} \cdot \alpha \cdot \mathbf{B} = \alpha \cdot \mathbf{A} \cdot \mathbf{B}, \quad (5.7)$$

$$\mathbf{A} \cdot \mathbf{B} \neq \mathbf{B} \cdot \mathbf{A}, \quad (5.8)$$

$$\text{Commutator } [\mathbf{A}, \mathbf{B}] = \mathbf{A} \cdot \mathbf{B} - \mathbf{B} \cdot \mathbf{A}, \quad (5.9)$$

$$\text{Identity } \mathbf{A} \cdot \mathbf{I} = \mathbf{A},$$

(5.10)

$$\text{Schwarz inequality [4]} \quad (|\langle x | \mathbf{A} | y \rangle|)^2 \leq \langle x | \mathbf{A} | x \rangle \cdot \langle y | \mathbf{A} | y \rangle \quad (5.11)$$

$$\text{Bessel inequality [4]} \quad \sum_{\alpha} [(\langle x_{\alpha} | x \rangle)]^2 \leq \langle x | x \rangle \quad \forall | x \rangle (\forall | x_{\alpha} \rangle \neq 0) (\in) L \quad (5.12)$$

$$\text{Parseval Theorem [4]} \quad \sum_{\alpha} (|\langle x_{\alpha} | x \rangle|)^2 = \langle x | x \rangle \quad (5.13)$$

Time evolution operator

**Time evolution operator** (conservative system, the Hamiltonian  $\mathbf{H}$ , is constant in time):

$$\mathbf{U}(t, t_0) = e^{-i \cdot \frac{\mathbf{H} \cdot (t-t_0)}{\hbar}} \quad \mathbf{U}(t_0, t_0) = 1 \quad (5.14)$$

$$\text{Differentiation: } \frac{\partial}{\partial t} \mathbf{U}(t, t_0) = -\frac{\mathbf{H} \cdot e^{-i \frac{\mathbf{H} \cdot (t-t_0)}{\hbar}} \cdot i}{\hbar} = \frac{-i}{\hbar} \cdot \mathbf{H} \cdot \mathbf{U}(t, t_0)$$

If  $\mathbf{H}$  is time independent then:  $i \cdot \hbar \cdot \frac{d}{dt} \mathbf{U}(t, t_0) = \mathbf{H} \cdot \mathbf{U}(t, t_0)$  (5.15)

Integral equation  $\mathbf{U}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t \mathbf{H} \cdot \mathbf{U}(\tau, t_0) d\tau$  (5.16)

Assuming a linear dependence of  $|\Psi(t)\rangle$  from  $|\Psi(t_0)\rangle$  I can write:

$$|\Psi(t)\rangle = \mathbf{U}(t, t_0) |\Psi(t_0)\rangle \quad (5.17)$$

$$\text{Differentiation: } \frac{d}{dt} |\Psi(t)\rangle = \left( \frac{d}{dt} \mathbf{U}(t, t_0) \right) |\Psi(t_0)\rangle \quad (5.18)$$

from (5.19) I get  $\frac{d}{dt} \mathbf{U}(t, t_0) = \frac{-i}{\hbar} \cdot \mathbf{H} \cdot \mathbf{U}(t, t_0)$ , which substituted in (5.22) gives:

$$\frac{d}{dt} |\Psi(t)\rangle = \frac{-i}{\hbar} \cdot \mathbf{H} \cdot \mathbf{U}(t, t_0) |\Psi(t_0)\rangle \quad (5.19)$$

that is the **Schrödinger equation**:

$$\frac{d}{dt} |\Psi(t)\rangle = \frac{-i}{\hbar} \cdot \mathbf{H} |\Psi(t)\rangle \quad (5.20)$$

Time evolution operator

## 6 Inverse operators

Given the operator  $\mathbf{A}$ , its inverse operator is indicated:  $\mathbf{A}^{-1}$ . It is an operator such that the product

$$\mathbf{A}^{-1} \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{A}^{-1} = \mathbf{I}, \quad (6.1)$$

where  $\mathbf{I}$  is the identity operator.

This property is not always verified (not invertible operator). That is the operator  $\mathbf{A}$  is invertible if and only if:

$$\forall |y\rangle \in \mathbf{R}(\mathbf{A}) \exists |x\rangle \in \mathbf{D}_{\mathbf{A}} \Rightarrow \mathbf{A}|x\rangle = |y\rangle \in \mathbf{R}(\mathbf{A}) \subset \mathbb{H}_2.$$

$$\mathbf{A}|x\rangle = |y\rangle \Rightarrow (\mathbf{A}^{-1} \cdot \mathbf{A})|x\rangle = |x\rangle = \mathbf{A}^{-1}|y\rangle.$$

$$(\mathbf{A} \cdot \mathbf{B})^{-1} = \mathbf{B}^{-1} \cdot \mathbf{A}^{-1}$$

The inverse of an operator can be found studying the equation  $\mathbf{A}|x\rangle = |0\rangle$ .

$$\forall \mathbf{A}, \mathbf{B} \in \text{Mat}(N, N) \Rightarrow (\mathbf{A} - \mathbf{B})^{-1} = \mathbf{A}^{-1} + \mathbf{A}^{-1} \cdot \mathbf{B} \cdot (\mathbf{A} - \mathbf{B})^{-1}. \quad (6.2)$$

$$\forall \mathbf{A}, \mathbf{B} \in \text{Mat}(N, N) \Rightarrow (\mathbf{A} - \mathbf{B})^{-1} - \mathbf{A}^{-1} \cdot \mathbf{B} \cdot (\mathbf{A} - \mathbf{B})^{-1} = \mathbf{A}^{-1}$$

$$\forall \mathbf{A}, \mathbf{B} \in \text{Mat}(N, N) \Rightarrow (\mathbf{I} - \mathbf{A}^{-1} \cdot \mathbf{B}) \cdot (\mathbf{A} - \mathbf{B})^{-1} = \mathbf{A}^{-1}$$

$$\forall \mathbf{A}, \mathbf{B} \in \text{Mat}(N, N) \Rightarrow (\mathbf{A} - \mathbf{B})^{-1} = (\mathbf{I} - \mathbf{A}^{-1} \cdot \mathbf{B})^{-1} \cdot \mathbf{A}^{-1}$$

$$\forall \mathbf{A}, \mathbf{B} \in \text{Mat}(N, N) \Rightarrow (\mathbf{A} - \mathbf{B})^{-1} = \mathbf{A}^{-1} \cdot [\mathbf{I} + \mathbf{B} \cdot (\mathbf{A} - \mathbf{B})^{-1}]$$

$$\forall \mathbf{A}, \mathbf{B} \in \text{Mat}(N, N) \Rightarrow (\mathbf{A} + \mathbf{B})^{-1} = (\mathbf{I} + \mathbf{A}^{-1} \cdot \mathbf{B})^{-1} \cdot \mathbf{A}^{-1}$$

$$\forall \mathbf{A}, \mathbf{B} \in \text{Mat}(N, N) \Rightarrow (\mathbf{A}^2 - \mathbf{B}^2)^{-1} = [(\mathbf{A} + \mathbf{B}) \cdot (\mathbf{A} - \mathbf{B}) + [\mathbf{A}, \mathbf{B}]]^{-1}$$

$$\forall \mathbf{A}, \mathbf{B} \in \text{Mat}(N, N) \Rightarrow (\mathbf{A}^2 + \mathbf{B}^2)^{-1} = [(\mathbf{A} + i\mathbf{B}) \cdot (\mathbf{A} - i\mathbf{B}) + i([\mathbf{A}, \mathbf{B}])]^{-1}$$

The operator  $\mathbf{P} = |u\rangle \langle v|$  has no inverse.

### Examples

$$\mathbf{A} := \begin{pmatrix} 1 & 2j & 3 \\ 4 & -5 & 6 \\ 7 & 8 & 9j \end{pmatrix} \quad \mathbf{B} := \begin{pmatrix} -1 & 2 & 4 \\ 5 & 8 & 0 \\ 6 & 4 & -1+j \end{pmatrix} \quad \mathbf{I} := \text{identity}(\text{rows}(\mathbf{A}))$$

Verify the following:  $(\mathbf{A} - \mathbf{B})^{-1} = \mathbf{A}^{-1} + \mathbf{A}^{-1} \cdot \mathbf{B} \cdot (\mathbf{A} - \mathbf{B})^{-1} = \mathbf{A}^{-1} \cdot [\mathbf{I} + \mathbf{B} \cdot (\mathbf{A} - \mathbf{B})^{-1}]$

$$(\mathbf{A} - \mathbf{B})^{-1} = \begin{pmatrix} 0.46 + 0.07j & -0.08 + 0.02j & 0.01 - 0.12j \\ -0.04 + 0.01j & -0.07 - 0.02j & 0.02 - 0.04j \\ -0.02 + 0.03j & 0.01 - 0.04j & 0.05 - 0.11j \end{pmatrix}$$

$$\mathbf{A}^{-1} \cdot [\mathbf{I} + \mathbf{B} \cdot (\mathbf{A} - \mathbf{B})^{-1}] = \begin{pmatrix} 0.46 + 0.07j & -0.08 + 0.02j & 0.01 - 0.12j \\ -0.04 + 0.01j & -0.07 - 0.02j & 0.02 - 0.04j \\ -0.02 + 0.03j & 0.01 - 0.04j & 0.05 - 0.11j \end{pmatrix}$$

Verify the following:  $(\mathbf{A} - \mathbf{B})^{-1} = (\mathbf{I} - \mathbf{A}^{-1} \cdot \mathbf{B})^{-1} \cdot \mathbf{A}^{-1}$

$$(\mathbf{I} - \mathbf{A}^{-1} \cdot \mathbf{B})^{-1} \cdot \mathbf{A}^{-1} = \begin{pmatrix} 0.46 + 0.07j & -0.08 + 0.02j & 0.01 - 0.12j \\ -0.04 + 0.01j & -0.07 - 0.02j & 0.02 - 0.04j \\ -0.02 + 0.03j & 0.01 - 0.04j & 0.05 - 0.11j \end{pmatrix}$$

Verify the following:  $(\mathbf{A}^2 - \mathbf{B}^2)^{-1} = [(\mathbf{A} + \mathbf{B}) \cdot (\mathbf{A} - \mathbf{B}) + [\mathbf{A}, \mathbf{B}]]^{-1}$

$$(\mathbf{A}^2 - \mathbf{B}^2)^{-1} = \begin{pmatrix} -0.58 - 0.21j & 0.33 - 0.2j & -0.04 + 0.07j \\ 0.23 - 0.31j & 0.06 + 0.24j & -0.04 - 0.04j \\ 0.02 + 0.13j & -0.08 - 0.06j & 0.02 + 0j \end{pmatrix}$$

$$[(\mathbf{A} + \mathbf{B}) \cdot (\mathbf{A} - \mathbf{B}) + \mathbf{A} \cdot \mathbf{B} - \mathbf{B} \cdot \mathbf{A}]^{-1} = \begin{pmatrix} -0.58 - 0.21j & 0.33 - 0.2j & -0.04 + 0.07j \\ 0.23 - 0.31j & 0.06 + 0.24j & -0.04 - 0.04j \\ 0.02 + 0.13j & -0.08 - 0.06j & 0.02 + 0j \end{pmatrix}$$

Verify the following:  $(\mathbf{A}^2 + \mathbf{B}^2)^{-1} = [(\mathbf{A} + i\mathbf{B}) \cdot (\mathbf{A} - i\mathbf{B}) + i([\mathbf{A}, \mathbf{B}])]^{-1}$

$$(\mathbf{A}^2 + \mathbf{B}^2)^{-1} = \begin{pmatrix} 0.02 + 0j & -0.01 - 0j & 0 - 0.01j \\ -0.01 + 0.01j & 0.01 - 0j & 0 - 0j \\ -0.01 - 0.01j & 0.01 - 0j & 0.01 + 0.01j \end{pmatrix}$$

$$[(\mathbf{A} + i\mathbf{B}) \cdot (\mathbf{A} - i\mathbf{B}) + i(\mathbf{A} \cdot \mathbf{B} - \mathbf{B} \cdot \mathbf{A})]^{-1} = \begin{pmatrix} 0.02 + 0j & -0.01 - 0j & 0 - 0.01j \\ -0.01 + 0.01j & 0.01 - 0j & 0 - 0j \\ -0.01 - 0.01j & 0.01 - 0j & 0.01 + 0.01j \end{pmatrix}$$

$$(\mathbf{A}^2 + \mathbf{B}^2)^{-1} = [(\mathbf{A} + i\mathbf{B}) \cdot (\mathbf{A} - i\mathbf{B}) + i(\mathbf{A} \cdot \mathbf{B} - \mathbf{B} \cdot \mathbf{A})]^{-1} \text{ simplify } \rightarrow 1$$

Examples of linear operators inversion:

$$\text{Fourier } \mathbf{F} = \int_{-\infty}^{\infty} e^{-i \cdot \omega \cdot x} dx$$

$$\mathbf{F}|f(x)\rangle = \int_{-\infty}^{\infty} e^{-i \cdot \omega \cdot x} |f(x)\rangle dx = |F(\omega)\rangle$$

$$\mathbf{F}^{-1} = \int_{-\infty}^{\infty} e^{i \cdot \omega \cdot x} dx$$

$$\mathbf{F}^{-1}|F(\omega)\rangle = \frac{1}{2 \cdot \pi} \cdot \int_{-\infty}^{\infty} e^{i \cdot \omega \cdot x} |F(\omega)\rangle d\omega = |f(x)\rangle$$

$$\text{Laplace } \mathcal{L} = \int_{-\infty}^{\infty} e^{-s \cdot x} dx \quad \text{use with the Mathcad prefix operator}$$



$$\mathcal{L} |g(x)\rangle = \int_{-\infty}^{\infty} e^{-s \cdot x} |g(x)\rangle dx = |G(s)\rangle$$

$$\mathcal{L}^{-1} |G(s)\rangle = \frac{1}{2 \cdot \pi \cdot i} \int_{\sigma-i \cdot \infty}^{\sigma+i \cdot \infty} e^{s \cdot x} ds |G(s)\rangle = |g(x)\rangle$$

### Differential operators Examples

$$D_{01}) \quad \mathbf{A} = -i \cdot \frac{\partial}{\partial x} \Rightarrow \mathbf{A}^{-1} = i \int \cdot dx + C$$

$$\mathbf{A} \cdot \mathbf{A}^{-1} = -i \cdot \frac{\partial}{\partial x} \left( -\frac{1}{i} \int \cdot dx + C \right) = \mathbf{I} \Rightarrow C = 0$$

$$\mathbf{A}^{-1} \cdot \mathbf{A} = \left( -\frac{1}{i} \int \cdot dx \right) \left( -i \cdot \frac{\partial}{\partial x} \right) = \int \cdot dx \frac{\partial}{\partial x} = \mathbf{I}$$

$$D_A \in \mathbb{R} \quad D_{02}) \quad \mathbf{A} = -\frac{\partial^2}{\partial x^2} = -i \cdot \frac{\partial}{\partial x} \left( -i \cdot \frac{\partial}{\partial x} \right)$$

$$\mathbf{A}^{-1} = \left( -i \cdot \frac{\partial}{\partial x} \right)^{-1} \left( -i \cdot \frac{\partial}{\partial x} \right)^{-1} = \left( -\frac{1}{i} \int \cdot dx \right) \left( -\frac{1}{i} \int \cdot dx \right) = - \int \cdot dx \int \cdot dx$$

$$\mathbf{A}^{-1} = - \int \int \cdot dx dx$$

Example with matrices

## 7 Adjoint operator [4]

The **adjoint** of a linear operator  $\mathbf{A}$  (or Hermitian conjugate operator of  $\mathbf{A}$ ) is written with a sword apex that is:

$$\mathbf{A}^\dagger$$

(read: adjoint of  $\mathbf{A}$ ).

$$\text{if } \mathbf{A} \in \text{MAT}(n, n): \mathbf{A}^\dagger = (\mathbf{A}^*)^T, \quad (7.1)$$

furthermore, the operator  $\mathbf{A}$  is **Hermitian** if and only if:  $\mathbf{A} = \mathbf{A}^\dagger$ ,

is anti Hermitian if:

$$\mathbf{A} = -\mathbf{A}^\dagger.$$

Let  $\mathbf{A}$  be a linear operator and  $|x\rangle$  the ket conjugated of the bra  $(\langle y | \mathbf{A})$ , namely  $|x\rangle = (\langle y | \mathbf{A})^*$ .

The ket  $|x\rangle$  depends anti linearly upon the bra  $\langle y |$ , it is therefore, a linear function of  $|y\rangle$ , through the new

operator  $\mathbf{A}^\dagger$ :

$$|x\rangle = \mathbf{A}^\dagger |y\rangle \quad (7.2)$$

From (2.4):  $\langle x | y \rangle = \langle y | x \rangle^*$ , it follows that:

$$\langle y | \mathbf{A} | x \rangle^* = \langle x | \mathbf{A}^\dagger | y \rangle. \quad (7.3)$$

The ket conjugated to  $\langle x | \mathbf{A}^\dagger$  is  $\mathbf{A} | x \rangle$ , (that is  $(\langle x | \mathbf{A}^\dagger)^* = \mathbf{A} | x \rangle$ ).

practical rule to obtain the adjoint (or Hermitian conjugate)

of a const replace with const\* complex conjugated of const.

of  $\langle x |$  replace with  $|x\rangle = \langle x |^\dagger$

of  $|x\rangle$  replace with  $\langle x | = |x\rangle^\dagger$

of  $\mathbf{A}$  replace with  $\mathbf{A}^\dagger$

of  $(c \cdot \mathbf{A})^\dagger$  replace with  $c^* \cdot \mathbf{A}^\dagger$  where c is a complex constant (7.4)

Reverse in each term the order of the various symbols:

$$(\mathbf{A} \mathbf{B})^\dagger = \mathbf{B}^\dagger \cdot \mathbf{A}^\dagger$$

$$\mathbf{D} = \mathbf{B} \mathbf{C} \quad (\mathbf{A} \mathbf{B} \mathbf{C})^\dagger = (\mathbf{A} \mathbf{D})^\dagger = \mathbf{D}^\dagger \mathbf{A}^\dagger = (\mathbf{B} \mathbf{C})^\dagger \mathbf{A}^\dagger = \mathbf{C}^\dagger \mathbf{B}^\dagger \mathbf{A}^\dagger$$

$$(\mathbf{A} | x \rangle)^\dagger = \langle x | \mathbf{A}^\dagger \quad (7.5)$$

$$\langle x | \mathbf{A} | y \rangle^\dagger = \langle y | \mathbf{A}^\dagger | x \rangle \quad (7.6)$$

$$(\mathbf{A} \mathbf{B} | x \rangle \langle y | \mathbf{C})^\dagger = \mathbf{C}^\dagger | y \rangle \langle x | \mathbf{B}^\dagger \mathbf{A}^\dagger \quad (7.7)$$

$$(\mathbf{A} \mathbf{B} | x \rangle \langle y | w \rangle)^\dagger = \langle w | y \rangle \langle x | \mathbf{B}^\dagger \mathbf{A}^\dagger \quad (7.8)$$

$$(\langle x | \mathbf{A} \mathbf{B} | y \rangle \langle y | w \rangle)^\dagger = \langle w | y \rangle \langle y | \mathbf{B}^\dagger \mathbf{A}^\dagger | x \rangle \quad (7.9)$$

$$(\langle x | \mathbf{A} \mathbf{B} | y \rangle \langle y | \mathbf{C} | w \rangle)^* = \langle w | \mathbf{C}^\dagger | y \rangle \langle y | \mathbf{B}^\dagger \mathbf{A}^\dagger | x \rangle \quad (7.10)$$

$$(\langle x | \mathbf{A} \mathbf{B} | y \rangle \langle v | \mathbf{C} | w \rangle)^* = \langle x | \mathbf{A} \mathbf{B} | y \rangle^* \cdot \langle v | \mathbf{C} | w \rangle^* \quad (7.11)$$

$$(\langle x | \mathbf{A} \mathbf{B} | y \rangle)^\dagger = \langle y | \mathbf{B}^\dagger \mathbf{A}^\dagger | x \rangle \quad (7.12)$$

$$(\langle x | \mathbf{C} | y \rangle)^\dagger = \langle y | \mathbf{C}^\dagger | x \rangle \quad (7.13)$$

$$\langle x | \mathbf{A} | y \rangle^* = \langle x | \mathbf{A} | y \rangle^\dagger = \langle y | \mathbf{A}^\dagger | x \rangle$$

A way to calculate the adjoint of a given operator  $\mathbf{A} \in L^2[a, b]$  (Hilbert space), that is  $\mathbf{A}^\dagger$ , is to calculate its expectation value, considering two vectors  $\langle u |$  and  $| v \rangle$ , as follows:

For  $L^2[a, b]$  the scalar product is 
$$\langle u | v \rangle = \int_a^b u(x)^* \cdot v(x) dx \quad (7.14)$$

example:  $u(x) := \alpha \cdot e^{j \cdot \omega \cdot x} \quad v(x) := \beta \cdot e^{j \cdot (\omega_1 \cdot x + \delta)}$

$$\langle u | v \rangle = \int_a^b u(x)^* \cdot v(x) dx = \alpha^* \cdot \beta \cdot \int_a^b e^{-j \cdot \omega \cdot x} \cdot e^{j \cdot (\omega_1 \cdot x + \delta)} dx = \alpha^* \cdot \beta \cdot \frac{\beta \cdot \alpha \cdot e^{\delta \cdot i} \cdot [e^{b \cdot j \cdot (\omega_1 - \omega)} - e^{a \cdot j \cdot (\omega_1 - \omega)}]}{\omega - \omega_1} \cdot i$$

example:  $u(x) := \alpha \cdot e^{j \cdot \omega \cdot x} \quad v(x) := \beta \cdot e^{j \cdot (\omega_1 \cdot x + \delta)} \quad \mathbf{A} = \frac{\partial}{\partial x}$

$$\langle u | \mathbf{A} | v \rangle = \int_a^b u(x)^* \cdot \mathbf{A} v(x) dx = \int_a^b u(x)^* \cdot \frac{\partial}{\partial x} v(x) dx = \alpha^* \cdot \beta \cdot \omega_1 \cdot j \cdot \int_a^b e^{-j \cdot \omega \cdot x} \cdot e^{j \cdot (\delta + \omega_1 \cdot x)} dx$$

$$\alpha^* \cdot \beta \cdot \omega_1 \cdot j \cdot \left[ \int_a^b e^{-j \cdot \omega \cdot x} \cdot e^{j \cdot (\delta + \omega_1 \cdot x)} dx \right] = \alpha^* \cdot \beta \cdot \omega_1 \cdot \frac{e^{\delta \cdot i} \cdot [e^{b \cdot j \cdot (\omega_1 - \omega)} - e^{a \cdot j \cdot (\omega_1 - \omega)}]}{\omega_1 - \omega}$$

$$\int_a^b u(x)^* \cdot \mathbf{A} v(x) dx = \alpha^* \cdot \beta \cdot \omega_1 \cdot \frac{e^{\delta \cdot i} \cdot [e^{b \cdot j \cdot (\omega_1 - \omega)} - e^{a \cdot j \cdot (\omega_1 - \omega)}]}{\omega_1 - \omega}$$

$$\langle u | \mathbf{A} | v \rangle = \alpha^* \cdot \beta \cdot \omega_1 \cdot \frac{e^{\delta \cdot i} \cdot [e^{b \cdot j \cdot (\omega_1 - \omega)} - e^{a \cdot j \cdot (\omega_1 - \omega)}]}{\omega_1 - \omega}$$

Search of the adjoint operator:

$$\langle u | \mathbf{A} | v \rangle^* = \langle u | \mathbf{A} | v \rangle^\dagger = \langle v | \mathbf{A}^\dagger | u \rangle = \left( \int_a^b u(x)^* \cdot \mathbf{A} v(x) dx \right)^* \quad \mathbf{A} \in L^2[a, b]$$

$$\langle v | \mathbf{A}^\dagger | u \rangle = \left( \int_a^b u(x)^* \cdot \mathbf{A} v(x) dx \right)^* \quad \mathbf{A} \in L^2[a, b] \quad (7.15)$$

For the integration by parts I consider: as finite factor:  $u^*$ , and as differential factor:  $\mathbf{A} v \cdot dx$ , I get:

$$\mathbf{A} \in L^2[a, b] \quad \int u(x)^* \cdot \mathbf{A} v(x) dx = u(x)^* \cdot \int \mathbf{A} v dx - \int \left( \int \mathbf{A} v dx \right) du^* \quad (7.16)$$

for the definite integral between a and b, I get:

$$\int_a^b u(x)^* \cdot \mathbf{A} v(x) dx = \left[ \lim_{x \rightarrow b} \left( u^* \cdot \int \mathbf{A} v dx \right) - \lim_{x \rightarrow a} \left( u^* \cdot \int \mathbf{A} v dx \right) \right] - \int_a^b \left( \int \mathbf{A} v dx \right) du^*$$

while taking into account the adjoint operator I have:

$$\langle v | \mathbf{A}^\dagger | u \rangle = \left( \int_a^b u(x)^* \cdot \mathbf{A} v(x) dx \right)^*$$

that is:

$$\left( \int_a^b u(x)^* \cdot \mathbf{A} v(x) dx \right)^* = \lim_{x \rightarrow b} \left( u^* \cdot \int \mathbf{A} v dx \right)^* - \lim_{x \rightarrow a} \left( u^* \cdot \int \mathbf{A} v dx \right)^* - \left[ \int_a^b \left( \int \mathbf{A} v dx \right) du^* \right]^*$$

$$\text{if } \lim_{x \rightarrow b} \left( u^* \cdot \int \mathbf{A} v dx \right)^* - \lim_{x \rightarrow a} \left( u^* \cdot \int \mathbf{A} v dx \right)^* = 0 \text{ then}$$

$$\langle v | \mathbf{A}^\dagger | u \rangle = \left( \int_a^b u(x)^* \cdot \mathbf{A} v(x) dx \right)^* = - \left[ \int_a^b \left( \int \mathbf{A} v dx \right) du^* \right]^*$$

1) Consider first the case where the operator is  $\mathbf{A} = c \cdot \mathbf{R}$ ,  $c \in \mathbb{C}$ ,  $\mathbf{R}$  be the vector Operator,

$$\mathbf{A}^\dagger = c^* \cdot \mathbf{R}^\dagger \quad (7.17)$$

$$\text{integrating by parts } \int_a^b u(x)^* \cdot \mathbf{A} v(x) dx = c \cdot \int_a^b u(x)^* \cdot \mathbf{R} v(x) dx, \quad \mathbf{A} \in (L^2[a, b])$$

Finite factor  $u^*$ , differential factor:  $\mathbf{R} v \cdot dx$  I get:

$$\langle v | \mathbf{A}^\dagger | u \rangle = \left( c \cdot \int u^* \cdot \mathbf{R} v dx \right)^* = c^* \cdot \left( \int u^* \cdot \mathbf{R} v dx \right)^* - \left[ \int \left( \int \mathbf{R} v dx \right) du^* \right]^*$$

$$\mathbf{A} \in L^2[a, b]$$

$$\langle v | A^\dagger | u \rangle = c \cdot \left[ \lim_{x \rightarrow b} \left( u^* \cdot \int \mathbf{R} v dx \right)^* - \lim_{x \rightarrow a} \left( u^* \cdot \int \mathbf{R} v dx \right)^* - \left[ \int_a^b \left( \int \mathbf{R} v dx \right) du^* \right]^* \right]$$

2)  $A = Q \cdot R$ ,  $(Q, R) \in L^2[a, b]$  are two vector Operators

$$\langle u | A | v \rangle^* = \langle u | A | v \rangle^\dagger = \langle v | A^\dagger | u \rangle = \left( \int_a^b u(x) \cdot Q R v(x) dx \right)^* \quad (Q, R) \in L^2[a, b]$$

$$\langle u | A | v \rangle^\dagger = \langle v | (QR)^\dagger | u \rangle = \langle v | R^\dagger Q^\dagger | u \rangle$$

$$\langle v | R^\dagger Q^\dagger | u \rangle = \int v^* \cdot R^\dagger Q^\dagger u dx = v^* \cdot \int R^\dagger Q^\dagger u dx - \int \left( \int R^\dagger Q^\dagger u dx \right) dv^*$$

calculate

$$\langle u | A | v \rangle^\dagger \text{ assuming that } (u, v) \in L^2[a, b] \quad \forall x \in [a, b] \quad u(a) = u(b) = 0$$

$$\begin{aligned} \langle v | R^\dagger Q^\dagger | u \rangle &= \lim_{x \rightarrow b} \left( v^* \cdot \int R^\dagger Q^\dagger u dx \right) - \lim_{x \rightarrow a} \left( v^* \cdot \int R^\dagger Q^\dagger u dx \right) \dots \\ &\quad + \int_a^b \left( - \int R^\dagger Q^\dagger u dx \right) dv^* \end{aligned}$$

3)  $A = F(x) \cdot R$ ,  $R$  be the given vectorial Operator,

calculate  $\langle u | A | v \rangle^\dagger$  assuming that  $(F(x), u, v) \in L^2[a, b] \quad \forall x \in [a, b] \quad u(a) = u(b) = 0$

$$\langle u | A | v \rangle^\dagger = \langle v | A^\dagger | u \rangle \quad A^\dagger = (F \cdot R)^\dagger = F^* \cdot R^\dagger$$

$$\langle v | (F^* \cdot R^\dagger) | u \rangle = \int v^* \cdot F^* \cdot R^\dagger u dx = v^* \cdot \int F^* \cdot R^\dagger u dx - \int \left( \int F^* \cdot R^\dagger u dx \right) dv^*$$

$$\langle v | (F^* \cdot R^\dagger) | u \rangle = \left[ \lim_{x \rightarrow b} \left( v^* \cdot \int F^* \cdot R^\dagger u dx \right) - \lim_{x \rightarrow a} \left( v^* \cdot \int F^* \cdot R^\dagger u dx \right) \dots \right. \\ \left. + \int_a^b \left( -v^* \cdot \int F^* \cdot R^\dagger u dx \right) dv^* \right]$$

4)  $A = Q + R$ ,  $A \in L^2[a, b]$   $Q, R$  be two vector Operators

$$\langle v | (Q^\dagger + R^\dagger) | u \rangle = \int v^* \cdot (Q^\dagger + R^\dagger) u dx = v^* \cdot \int (Q^\dagger + R^\dagger) u dx - \int \left[ \int (Q^\dagger + R^\dagger) v dx \right] dv^*$$

$A \in L^2[a, b]$

$$\begin{aligned} \langle v | (Q^\dagger + R^\dagger) | u \rangle &= \lim_{x \rightarrow b} \left[ v^* \cdot \int (Q^\dagger + R^\dagger) u dx \right] \dots \\ &\quad + (-1) \cdot \lim_{x \rightarrow a} \left[ v^* \cdot \int (Q^\dagger + R^\dagger) u dx \right] - \int_a^b \left[ v^* \cdot \int (Q^\dagger + R^\dagger) u dx \right] dv^* \end{aligned}$$

## 8 Examples of adjoint operators calculation

### Example Adj<sub>1</sub>) [8]

given the operator  $\mathbf{A} = -i \cdot \frac{\partial}{\partial x}$

calculate  $\langle u | \mathbf{A}^\dagger | v \rangle$  assuming that  $(u, v) \in L^2[a, b] \quad \forall x \in [a, b] \quad u(a) = u(b) = 0$

according to the definition:  $\langle v | \mathbf{A}^\dagger | u \rangle = \left( \langle u | -i \cdot \frac{\partial}{\partial x} | v \rangle \right)^* = \left( i \cdot \int_a^b u(x)^* \frac{\partial}{\partial x} v(x) dx \right)^*$

Integration by parts (finite factor:  $u(x)^*$ , differential factor:  $\frac{\partial}{\partial x} v(x)$ ):

$$\left( i \cdot \int_a^b u(x)^* \frac{\partial}{\partial x} v(x) dx \right)^* = \left[ i \cdot u(x)^* \cdot \int_a^b \frac{\partial}{\partial x} v(x) dx - i \cdot \int_a^b \left( \int_a^b \frac{\partial}{\partial x} v dx \right) du^* \right]^*$$

$$\langle v | \mathbf{A}^\dagger | u \rangle = \left[ -i \cdot \left[ \lim_{x \rightarrow b} \left[ u(x)^* \cdot \int \frac{\partial}{\partial x} v dx^* \right] - \lim_{x \rightarrow a} \left[ u(x)^* \cdot \int \frac{\partial}{\partial x} v dx^* \right] \right] + \left[ \int_a^b \left( - \int \frac{\partial}{\partial x} v dx \right) du^* \right]^* \right]$$

$$\langle v | \mathbf{A}^\dagger | u \rangle = -i \cdot \left[ \lim_{x \rightarrow b} (u \cdot v^*) - \lim_{x \rightarrow a} (u \cdot v^*) - \int_a^b \left( \int \frac{\partial}{\partial x} v dx \right) du^* \right]^*$$

$$i \cdot (v(b)^* \cdot u(b) - v(a)^* \cdot u(a)) = 0$$

$$\langle v | \mathbf{A}^\dagger | u \rangle = i \cdot (v(b)^* \cdot u(b) - v(a)^* \cdot u(a)) - \langle u | i \cdot \frac{\partial}{\partial x} | v \rangle$$

$$\langle v | \mathbf{A}^\dagger | u \rangle = -\langle u | i \cdot \frac{\partial}{\partial x} | v \rangle = \langle v | i \cdot \frac{\partial}{\partial x} | u \rangle$$

$$\langle v | \mathbf{A}^\dagger | u \rangle = \left( \langle u | i \cdot \frac{\partial}{\partial x} | v \rangle \right)^* = -i \cdot \left( \int_a^b v du^* \right)^* = -i \cdot \left[ \int_a^b v \cdot \frac{\partial}{\partial x} (u^*) dx \right]^* = -i \cdot \int_a^b v^* \cdot \frac{\partial}{\partial x} u dx$$

resulting adjoint operator  $\mathbf{A}^\dagger = i \cdot \frac{\partial}{\partial x} \quad \forall x \in ([a, b]) \quad u(a) = u(b) = 0$

$\mathbf{A}^\dagger = -\mathbf{A}$  *anti-Hermitian operator*

### Example Adj<sub>2</sub>) [1]

given the operator  $\mathbf{A}_x = P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x)$

with  $\boxed{P(x) \neq 0} \quad \boxed{Q(x) \neq 0} \quad \boxed{R(x) \neq 0}$

calculate  $\langle u | \mathbf{A}_x^\dagger | v \rangle$  assuming that  $(u, v) \in L^2[a, b] \quad \forall x \in [a, b] \quad u(a) = u(b) = 0$

$$\int_a^b u(x)^* \cdot \left( P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x) \right) v(x) dx = \int_a^b u(x)^* \mathbf{A}_x^\dagger v(x) dx$$

$$\int_a^b u(x)^* \cdot \left( P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x) \right) v(x) dx = \int_a^b \left( u(x)^* \cdot P(x) \cdot \frac{\partial^2}{\partial x^2} v(x) + u(x)^* \cdot R(x) \cdot \frac{\partial}{\partial x} v(x) + u(x)^* \cdot Q(x) \cdot v(x) \right) dx$$

$$\int_a^b \left( u(x)^* \cdot P(x) \cdot \frac{\partial^2}{\partial x^2} v(x) + u(x)^* \cdot R(x) \cdot \frac{\partial}{\partial x} v(x) + u(x)^* \cdot Q(x) \cdot v(x) \right) dx = \int_a^b \left( u(x)^* \cdot \left( P(x) \cdot \frac{\partial^2}{\partial x^2} + 2 \cdot \frac{\partial}{\partial x} P(x) \cdot \frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2} P(x) + R(x) \cdot \frac{\partial}{\partial x} + \frac{\partial}{\partial x} R(x) + Q(x) \right) v(x) \right) dx = \int_a^b u(x)^* \mathbf{A}_x^\dagger v(x) dx$$

$$\mathbf{A}_x^\dagger = P(x) \cdot \frac{\partial^2}{\partial x^2} + (2 \cdot P'(x) - R(x)) \cdot \frac{\partial}{\partial x} + (P''(x) - R'(x) + Q(x))$$

Adjoint operator of  $\mathbf{A}_x$ :  $\mathbf{A}_x^\dagger = \left( \frac{\partial^2}{\partial x^2} \right) P(x) - \left( \frac{\partial}{\partial x} \right) R(x) + Q(x)$  or more explicitly:

$$\mathbf{A}_x^\dagger = \left( \frac{\partial^2}{\partial x^2} \right) P(x) - \left( \frac{\partial}{\partial x} \right) R(x) + Q(x) = P(x) \cdot \frac{\partial^2}{\partial x^2} + (2 \cdot P'(x) - R(x)) \cdot \frac{\partial}{\partial x} + (P''(x) - R'(x) + Q(x))$$

**Example Adj<sub>3</sub>**

given the operator  $A = P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x)$

with  $P(x) \neq 0$   $Q(x) \neq 0$   $R(x) = \frac{\partial}{\partial x} P(x)$

$$A = P(x) \cdot \frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} P(x) \cdot \frac{\partial}{\partial x} + Q(x)$$

as seen the general adjoint is  $A_x^\dagger = P(x) \cdot \frac{\partial^2}{\partial x^2} + (2 \cdot P'(x) - R(x)) \cdot \frac{\partial}{\partial x} + (P''(x) - R'(x) + Q(x))$

substituting the data it become

$$A_x^\dagger = P(x) \cdot \frac{\partial^2}{\partial x^2} + \left( 2 \cdot \frac{\partial}{\partial x} P(x) - \frac{\partial}{\partial x} P(x) \right) \frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2} P(x) - \frac{\partial^2}{\partial x^2} P(x) + Q(x)$$

after a simplification the resulting adjoint operator is

$$A_x^\dagger = P(x) \cdot \frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} P(x) \cdot \frac{\partial}{\partial x} + Q(x) = P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x) = A$$

If  $R(x) = \frac{\partial}{\partial x} P(x) \Rightarrow A_x^\dagger = A$  *A is Hermitian*

**Example Adj<sub>4</sub>**

Assume  $Q(x) \neq 0$   $R(x) \neq 0$   $P(x) = 0$

$$A = P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x)$$

the operator is  $A = R(x) \cdot \frac{\partial}{\partial x} + Q(x)$

as seen the general adjoint is  $A_x^\dagger = P(x) \cdot \frac{\partial^2}{\partial x^2} + (2 \cdot P'(x) - R(x)) \cdot \frac{\partial}{\partial x} + (P''(x) - R'(x) + Q(x))$

substituting the data it become  $A_x^\dagger = -R(x) \cdot \frac{\partial}{\partial x} - R'(x) + Q(x)$

resulting adjoint operator  $A_x^\dagger = -R(x) \cdot \frac{\partial}{\partial x} - \frac{\partial}{\partial x} R(x) + Q(x)$

**Example Adj<sub>5</sub>**

$P(x) = 1$   $R(x) = 0$   $Q(x) = 0$

the operator  $A = P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x)$

$$A = \frac{\partial^2}{\partial x^2}$$

as seen the general adjoint is  $A_x^\dagger = P(x) \cdot \frac{\partial^2}{\partial x^2} + (2 \cdot P'(x) - R(x)) \cdot \frac{\partial}{\partial x} + (P''(x) - R'(x) + Q(x))$

substituting the data it become  $A_x^\dagger = \frac{\partial^2}{\partial x^2}$

resulting adjoint operator  $A = \frac{\partial^2}{\partial x^2} \Rightarrow A_x^\dagger = \frac{\partial^2}{\partial x^2} \Rightarrow A_x^\dagger = A$  *A is Hermitian*

**Example Adj<sub>6</sub>**

given the operator  $A = P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x)$

with  $P(x) = 0$   $R(x) = 1$   $Q(x) = 0$

$$A = \frac{\partial}{\partial x}$$

as seen the general adjoint is  $A_x^\dagger = P(x) \cdot \frac{\partial^2}{\partial x^2} + (2 \cdot P'(x) - R(x)) \cdot \frac{\partial}{\partial x} + (P''(x) - R'(x) + Q(x))$

substituting the data it become  $A_x^\dagger = 0 \cdot \frac{\partial^2}{\partial x^2} + (2 \cdot 0 - 1) \cdot \frac{\partial}{\partial x} + (0 - 0 + 0) = -\frac{\partial}{\partial x}$

resulting adjoint operator  $A = \frac{\partial}{\partial x} \Rightarrow A_x^\dagger = -\frac{\partial}{\partial x}$   $A_x^\dagger = -A$  *is anti Hermitian*

**Example Adj<sub>7</sub>**

given the operator  $A = -i \cdot \frac{\partial}{\partial x}$

$$A = P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x)$$

with  $P(x) = 0$   $R(x) = -i$   $Q(x) = 0$

$$A_x^\dagger = P(x) \cdot \frac{\partial^2}{\partial x^2} + \left( 2 \cdot \frac{\partial}{\partial x} P(x) - R(x) \right) \cdot \frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2} P(x) - \frac{\partial}{\partial x} R(x) + Q(x) = i \cdot \frac{\partial}{\partial x}$$

$$A^\dagger = 0 \cdot \frac{\partial^2}{\partial x^2} + \left[ 2 \cdot \frac{\partial}{\partial x} \cdot 0 - (-i) \right] \cdot \frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2} \cdot 0 - 0 + 0 = i \cdot \frac{\partial}{\partial x}$$

resulting adjoint operator  $A = -i \cdot \frac{\partial}{\partial x} \Rightarrow A^\dagger = i \cdot \frac{\partial}{\partial x} \quad A^\dagger = -A \quad \text{is anti Hermitian}$

### Example Adj<sub>8</sub>

given the operator  $A = P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x)$ ,

$$P(x) = -1 \quad R(x) = 0 \quad Q(x) = 0$$

$$A = -\frac{\partial^2}{\partial x^2}$$

$$A_x^\dagger = P(x) \cdot \frac{\partial^2}{\partial x^2} + (2 \cdot P'(x) - R(x)) \cdot \frac{\partial}{\partial x} + (P''(x) - R'(x) + Q(x))$$

$$A_x^\dagger = \left( \frac{\partial^2}{\partial x^2} \right) P(x) - \left( \frac{\partial}{\partial x} \right) R(x) + Q(x) = -\frac{\partial^2}{\partial x^2}$$

resulting adjoint operator  $A^\dagger = -\frac{\partial^2}{\partial x^2}$

$$A = A^\dagger$$

### Example Adj<sub>9</sub>

given the operator  $A = P(x) \cdot \frac{\partial^2}{\partial x^2} + R(x) \cdot \frac{\partial}{\partial x} + Q(x)$ ,

$$P(x) = 1 \quad R(x) \neq 0 \quad Q(x) \neq 0$$

The Wronskian is:  $W(\xi) = f_1(\xi) \cdot f_2(\xi) - f_2(\xi) \cdot f_1(\xi) = \left( \frac{\partial}{\partial x} f_1(\xi) \right) \cdot f_2(\xi) - \left( \frac{\partial}{\partial x} f_2(\xi) \right) \cdot f_1(\xi)$

it satisfy the differential equation  $A_x G(x, \xi) = \delta(x - \xi)$  where  $G(x, \xi)$  is the Green function:

$$G(x, \xi) = \begin{cases} \frac{u_1(x) \cdot u_2(\xi) - u_2(x) \cdot u_1(\xi)}{W(\xi)} & \text{if } \xi < x \\ 0 & \text{otherwise} \end{cases} \quad W(x) \text{ is the Wronskian}$$

For the variable  $\xi$  there is a second differential equation, namely:

$$A_\xi^\dagger G(x, \xi) = \delta(x - \xi)$$

resulting adjoint operator

$$A^\dagger = \frac{\partial^2}{\partial x^2} - R(x) \cdot \frac{\partial}{\partial x} - \frac{\partial}{\partial x} R(x) + Q(x)$$

### Example Adj<sub>10</sub>

$$A = \nabla^2 = \nabla \cdot \nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

since  $A = \frac{\partial^2}{\partial x^2} \Rightarrow A^\dagger = \frac{\partial^2}{\partial x^2} \Rightarrow A^\dagger = A \quad A \text{ is Hermitian}$

resulting adjoint operator  $A^\dagger = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2 \quad A = A^\dagger \quad A \text{ is Hermitian}$

$$(\nabla^2)^\dagger = \nabla^2 \quad \text{is auto-adjoint or Hermitian}$$

### Example Adj<sub>11</sub>

$$A = \nabla \cdot = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$$

since  $A = \frac{\partial}{\partial x} \Rightarrow A^\dagger = -\frac{\partial}{\partial x} \quad A^\dagger = -A$

resulting adjoint operator  $A^\dagger = -\left( \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \right) = -\nabla \cdot \quad A = -A^\dagger \quad A \text{ is anti Hermitian}$

$$(\nabla \cdot)^\dagger = -\nabla \cdot \quad \text{is anti Hermitian}$$

### Example Adj<sub>12</sub>

$$A = \nabla = \frac{\partial}{\partial x} \cdot \mathbf{i}_x + \frac{\partial}{\partial y} \cdot \mathbf{i}_y + \frac{\partial}{\partial z} \cdot \mathbf{i}_z$$

since  $A = \frac{\partial}{\partial x} \Rightarrow A^\dagger = -\frac{\partial}{\partial x} \quad A^\dagger = -A$

resulting adjoint operator  $A^\dagger = -\left( \frac{\partial}{\partial x} \cdot \mathbf{i}_x + \frac{\partial}{\partial y} \cdot \mathbf{i}_y + \frac{\partial}{\partial z} \cdot \mathbf{i}_z \right) = -\nabla \quad A = -A^\dagger \quad A \text{ is anti Hermitian}$

$$\nabla^\dagger = -\nabla \quad \text{is anti Hermitian}$$

### Example Adj<sub>13</sub>

$$A = \nabla \times$$

$$\mathbf{A}^\dagger = (\nabla \times)^\dagger$$

Explicit calculation:

$$(\nabla \times)^\dagger = \left[ \begin{array}{l} \left( \frac{\partial}{\partial y} A_0(x, y, z)_2 - \frac{\partial}{\partial z} A_0(x, y, z)_1 \right) \cdot \mathbf{i}_x \dots \\ + \left( \frac{\partial}{\partial z} A_0(x, y, z)_0 - \frac{\partial}{\partial x} A_0(x, y, z)_2 \right) \cdot \mathbf{i}_y \dots \\ + \left( \frac{\partial}{\partial x} A_0(x, y, z)_1 - \frac{\partial}{\partial y} A_0(x, y, z)_0 \right) \cdot \mathbf{i}_z \end{array} \right]^\dagger$$

$$\left[ \begin{array}{l} \left( \frac{\partial}{\partial y} A_0(x, y, z)_2 - \frac{\partial}{\partial z} A_0(x, y, z)_1 \right) \cdot \mathbf{i}_x \dots \\ + \left( \frac{\partial}{\partial z} A_0(x, y, z)_0 - \frac{\partial}{\partial x} A_0(x, y, z)_2 \right) \cdot \mathbf{i}_y \dots \\ + \left( \frac{\partial}{\partial x} A_0(x, y, z)_1 - \frac{\partial}{\partial y} A_0(x, y, z)_0 \right) \cdot \mathbf{i}_z \end{array} \right]^\dagger = \left[ \begin{array}{l} \left( \frac{\partial}{\partial y} A_0(x, y, z)_2 \right)^\dagger - \left( \frac{\partial}{\partial z} A_0(x, y, z)_1 \right)^\dagger \cdot \mathbf{i}_x \dots \\ + \left( \frac{\partial}{\partial z} A_0(x, y, z)_0 \right)^\dagger - \left( \frac{\partial}{\partial x} A_0(x, y, z)_2 \right)^\dagger \cdot \mathbf{i}_y \dots \\ + \left( \frac{\partial}{\partial x} A_0(x, y, z)_1 \right)^\dagger - \left( \frac{\partial}{\partial y} A_0(x, y, z)_0 \right)^\dagger \cdot \mathbf{i}_z \end{array} \right]$$

since  $\mathbf{A} = \frac{\partial}{\partial \mathbf{x}} \Rightarrow \mathbf{A}^\dagger = -\frac{\partial}{\partial \mathbf{x}}$  is anti Hermitian

$$\left( \frac{\partial}{\partial y} A_0(x, y, z)_2 \right)^\dagger = -\frac{\partial}{\partial y} A_0(x, y, z)_2$$

$$\left[ \begin{array}{l} \left( -\frac{\partial}{\partial y} A_0(x, y, z)_2 + \frac{\partial}{\partial z} A_0(x, y, z)_1 \right) \cdot \mathbf{i}_x \dots \\ + \left( \frac{\partial}{\partial z} A_0(x, y, z)_0 + \frac{\partial}{\partial x} A_0(x, y, z)_2 \right) \cdot \mathbf{i}_y \dots \\ + \left( \frac{\partial}{\partial x} A_0(x, y, z)_1 + \frac{\partial}{\partial y} A_0(x, y, z)_0 \right) \cdot \mathbf{i}_z \end{array} \right] = \left[ \begin{array}{l} \left( \frac{\partial}{\partial y} A_0(x, y, z)_2 - \frac{\partial}{\partial z} A_0(x, y, z)_1 \right) \cdot \mathbf{i}_x \dots \\ + \left( \frac{\partial}{\partial z} A_0(x, y, z)_0 - \frac{\partial}{\partial x} A_0(x, y, z)_2 \right) \cdot \mathbf{i}_y \dots \\ + \left( \frac{\partial}{\partial x} A_0(x, y, z)_1 - \frac{\partial}{\partial y} A_0(x, y, z)_0 \right) \cdot \mathbf{i}_z \end{array} \right]$$

$(\nabla \times)^\dagger = -\nabla \times$  is anti Hermitian

#### Example Adj<sub>14</sub>

$$\mathbf{A} = \left( \frac{\partial^2}{\partial x \partial y} \right)^\dagger$$

$$\mathbf{A}^\dagger = \left( \frac{\partial^2}{\partial x \partial y} \right)^\dagger = \left( \frac{\partial}{\partial x} \frac{\partial}{\partial y} \right)^\dagger = \left( \frac{\partial}{\partial y} \right)^\dagger \left( \frac{\partial}{\partial x} \right)^\dagger = \left( -\frac{\partial}{\partial y} \right) \left( -\frac{\partial}{\partial x} \right) = \frac{\partial^2}{\partial y \partial x}$$

$\mathbf{A} = \mathbf{A}^\dagger$  A is Hermitian

#### Example Adj<sub>15</sub>

$$\mathbf{A} = \nabla \nabla \cdot$$

calculations

$$(\nabla \nabla \cdot)^\dagger = (\nabla \cdot)^\dagger \nabla^\dagger$$

$$(\nabla \cdot)^\dagger = -\nabla \cdot$$

$$\nabla^\dagger = -\nabla$$

$$(\nabla \cdot)^\dagger \nabla^\dagger = -\nabla \cdot (-\nabla) = \nabla \cdot \nabla = \nabla^2$$

#### Example Adj<sub>16</sub>

Show that the operator  $\nabla \times \nabla \times$  is auto-adjoint or Hermitian:  $(\nabla \times \nabla \times)^\dagger = \nabla \times \nabla \times$

$$1) (\nabla \times \nabla \times)^\dagger = (\nabla \times)^\dagger (\nabla \times)^\dagger = (-\nabla \times) (-\nabla \times) = \nabla \times \nabla \times$$

$\mathbf{A} = \mathbf{A}^\dagger$  A is Hermitian

## 9 Spectral Decomposition of an Operator

Given the operator  $\mathbf{A}$  defined in  $D \in \mathbb{H}$ , I associate to it the operator  $\mathbf{A} - \lambda \cdot \mathbf{I}$ , where  $\mathbf{I}$  is the identity operator and  $\lambda$  is a complex number. I want calculate the inverse operator  $(\mathbf{A} - \lambda \cdot \mathbf{I})^{-1}$ . To do that, I consider the action of the operator on a ket such that:  $(\mathbf{A} - \lambda \cdot \mathbf{I}) |x\rangle = |0\rangle$  that is it must be satisfied the eigenvalue equation  $\mathbf{A} |x\rangle = \lambda |x\rangle$ .

It follows that the operator  $\mathbf{A} - \lambda \cdot \mathbf{I}$  is invertible if the solution  $|x\rangle$  of the eigenvalue equation is the simplest, that is a function of  $\lambda$ . The set of the complex values of  $\lambda$  for which the equation has a no banal solution, that is the values of  $\lambda$  for that the operator isn't invertible, forms the discrete spectrum of the operator  $\mathbf{A}$  and are the eigenvalues of  $\mathbf{A}$ .

Vice versa when the values of  $\lambda$  gives the banal solution, then the operator  $\mathbf{A} - \lambda \cdot \mathbf{I}$  is invertible that is  $\exists (\mathbf{A} - \lambda \cdot \mathbf{I})^{-1}$ . When this happens there are several possibilities:

- 1) if the operator  $(\mathbf{A} - \lambda \cdot \mathbf{I})^{-1}$  is limited, the corresponding value of  $\lambda$  belongs to the solving set of the operator  $\mathbf{A}$ .
- 2) if the operator  $(\mathbf{A} - \lambda \cdot \mathbf{I})^{-1}$  isn't limited, then  $\lambda$  belongs to the continuous spectrum of  $\mathbf{A}$ .

Consider the space  $(L = \{|x\rangle\}) \in \mathbb{H}$ . Each linear operator  $\mathbf{A}$  has its eigenvectors and the corresponding eigenvalues satisfying the equation:

$$\mathbf{A} |x\rangle = \lambda |x\rangle, \quad (9.1)$$

where the  $\lambda$  are numbers and are the eigenvalues of the operator  $\mathbf{A}$ , they constitute the set of the eigenvalues of the operator  $\mathbf{A}$ . To each eigenvector is associated an eigenvalue.

If there exist several linear independent eigenvectors belonging to the same eigenvalue  $\lambda$ , any linear combination of this kets is an eigenket of  $\mathbf{A}$  belonging to this  $\lambda$ . That is the ensemble of eigenvectors of  $\mathbf{A}$  belonging to  $\lambda$  forms a vector space called **the subspace of the eigenvalue**  $\lambda$ . If this subspace is one dimensional, the eigenvalue is said **single or non-degenerate**.

If this subspace is multidimensional, the eigenvalue is said **degenerate**. The order of degeneracy is given by the number of dimensions of this subspace (maybe of infinite order).

The auto bras and the corresponding eigenvalues of the operator  $\mathbf{A}$  satisfy the equation:

$$\langle y | \mathbf{A} = \langle y | \mu, \quad (9.2)$$

where the  $\mu$  are numbers and are other eigenvalues of the operator  $\mathbf{A}$ .  $\lambda$  and  $\mu$  constitutes the spectrum of  $\mathbf{A}$ .

Instead, if  $\mathbf{A}$  is Hermitian ( $\mathbf{A} = \mathbf{A}^\dagger$ ):

i) the two eigenvalues spectra are identical ( $\lambda = \mu$ ),

ii) all eigenvalues are real, (since  $\mathbf{A} = \mathbf{A}^\dagger$ ,  $\langle x | \mathbf{A} | x \rangle = \lambda \langle x | x \rangle$ ,

$$\langle x | \mathbf{A} | x \rangle^* = \langle x | \mathbf{A}^\dagger | x \rangle = \langle x | \mathbf{A} | x \rangle = (\lambda \langle x | x \rangle)^* = \lambda^* \langle x | x \rangle = \lambda \langle x | x \rangle,$$

$\langle x | \mathbf{A} | x \rangle$  and  $\langle x | x \rangle$  are real, therefore also  $\lambda$  is real.

iii) each auto ket and autobra correspond to the same eigenvalue  $\lambda = \mu$ . The subspace of the autobras of  $\mu$  is the dual space of the subspace of the eigenvectors of the same eigenvalue.

iv) Eigenvectors belonging to distinct eigenvalues are orthogonal.

Given  $\mathbf{A} |x\rangle = \lambda |x\rangle$  and  $\langle y | \mathbf{A} = \langle y | \mu$ ,  $\langle y | \mathbf{A} | x \rangle = \langle y | \lambda | x \rangle = \lambda \langle y | x \rangle$ ,

$$\langle y | \mathbf{A} = \langle y | \mu, \langle y | \mathbf{A} | x \rangle = \langle y | \mu | x \rangle = \mu \langle y | x \rangle,$$

subtracting term by term I get:  $\langle y | \mathbf{A} | x \rangle - \langle y | \mathbf{A} | x \rangle = 0 = (\lambda - \mu) \langle y | x \rangle$ , consequently if

$$\lambda \neq \mu, \langle y | x \rangle = 0.$$

Based on the property 2.8), the norms of the kets must be finite. The vectors with infinite norm with eigenvalues belonging to the **continuous spectrum** don't belong to the Hilbert space. Properties i), ii), iii), iv) are yet true.

## 10 Projector Operator [7]

Consider the Hilbert space  $\mathbb{H}$  and a subspace  $h \subseteq \mathbb{H}$ .  $h$  is linear and closed. The ket  $|x\rangle \in \mathbb{H}$  can be divided in two vectors:  $|x_s\rangle$  and  $|x_n\rangle$ , such that  $|x_s\rangle \in h$  and  $|x_n\rangle$  has the property to be orthogonal to each vector of  $h$ ,

that is  $\langle x_s | x_n \rangle = 0, \forall |x_s\rangle \in h$ . If the space  $h$  is closed under multiplication by a number and under vector addition, that is if  $|x\rangle$  and  $|y\rangle \in h$  and  $\alpha, \beta \in \mathbb{C}$ ,

$$\mathbf{P}(\alpha |x\rangle + \beta |y\rangle) = \alpha \mathbf{P} |x\rangle + \beta \mathbf{P} |y\rangle = \alpha |x\rangle + \beta |y\rangle$$

the decomposition exists and is unique. The operator that associates to each ket  $|x\rangle$  its  $|x_s\rangle$  is defined in the whole space  $\mathbb{H}$  and is the projector  $\mathbf{P}$ , that is:

$$\mathbf{P} |x\rangle = |x_s\rangle, \forall |x\rangle \in \mathbb{H}, \mathbf{P} \in \mathbb{H}.$$

**Properties:**  $\mathbf{P}$  is limited:  $\|\mathbf{P} |x\rangle\| \leq \| |x\rangle \|$   
(10.1)

$$\text{it is idempotent: } \mathbf{P}^2 = \mathbf{P} \quad (10.2)$$

$$\mathbf{P} |x\rangle = |x_s\rangle \quad (10.3)$$

$$\mathbf{P} \mathbf{P} |x\rangle = \mathbf{P} |x_s\rangle = |x_s\rangle \quad (10.4)$$

$$\text{It is auto-adjoint or Hermitian: } \mathbf{P} = \mathbf{P}^\dagger \quad \text{necessary and sufficient condition} \quad (10.3)$$

A Hermitian operator  $\mathbf{P}$  is called a **projection operator or projector** iff it is independent ( $\mathbf{P}^2 = \mathbf{P}$ ).

**Example 5:**

$$|a\rangle = \begin{pmatrix} 0.116 + 0.116i \\ 0.233 + 0.164i \\ 0.349 + 0.465i \\ 0.465 + 0.581i \end{pmatrix} \quad |b\rangle = \begin{pmatrix} 0.365 - 0.073i \\ 0.438 + 0.073i \\ 0.51 + 0.126i \\ 0.583 - 0.219i \end{pmatrix}$$

$$\langle a | a \rangle = (0.116 - 0.116i \ 0.233 - 0.164i \ 0.349 - 0.465i \ 0.465 - 0.581i) \cdot \begin{pmatrix} 0.116 + 0.116i \\ 0.233 + 0.164i \\ 0.349 + 0.465i \\ 0.465 + 0.581i \end{pmatrix} = 1$$

$|a\rangle$  is normalized to unit

$$\langle b | = (0.365 + 0.073i \ 0.438 - 0.073i \ 0.51 - 0.126i \ 0.583 + 0.219i)$$

$$\langle b | b \rangle = (0.365 + 0.073i \ 0.438 - 0.073i \ 0.51 - 0.126i \ 0.583 + 0.219i) \cdot \begin{pmatrix} 0.365 - 0.073i \\ 0.438 + 0.073i \\ 0.51 + 0.126i \\ 0.583 - 0.219i \end{pmatrix} = 1$$

$|b\rangle$  is normalized to unit



$$\langle a | b \rangle = (0.116 - 0.116i \quad 0.233 - 0.164i \quad 0.349 - 0.465i \quad 0.465 - 0.581i) \cdot \begin{pmatrix} 0.365 - 0.073i \\ 0.438 + 0.073i \\ 0.51 + 0.126i \\ 0.583 - 0.219i \end{pmatrix} = 0.528 - 0.739i$$

$|a\rangle$  and  $|b\rangle$  are normalized to unit but not orthogonal.

$$\mathbf{P} = |a\rangle\langle a| = \begin{pmatrix} 0.116 + 0.116i \\ 0.233 + 0.164i \\ 0.349 + 0.465i \\ 0.465 + 0.581i \end{pmatrix} \cdot (0.116 - 0.116i \quad 0.233 - 0.164i \quad 0.349 - 0.465i \quad 0.465 - 0.581i)$$

$$\mathbf{P} = |a\rangle\langle a| = \begin{pmatrix} \frac{1}{37} & 0.046 + 8.004i \times 10^{-3} & 0.094 - 0.013i & 0.121 - 0.013i \\ 0.046 - 8.004i \times 10^{-3} & \frac{3}{37} & 0.158 - 0.051i & 0.204 - 0.059i \\ 0.094 + 0.013i & 0.158 + 0.051i & \frac{24}{71} & 0.432 + 0.013i \\ 0.121 + 0.013i & 0.204 + 0.059i & 0.432 - 0.013i & \frac{5}{9} \end{pmatrix}$$

$$\mathbf{P}^\dagger = \begin{pmatrix} \frac{1}{37} & 0.046 + 8.004i \times 10^{-3} & 0.094 - 0.013i & 0.121 - 0.013i \\ 0.046 - 8.004i \times 10^{-3} & \frac{3}{37} & 0.158 - 0.051i & 0.204 - 0.059i \\ 0.094 + 0.013i & 0.158 + 0.051i & \frac{24}{71} & 0.432 + 0.013i \\ 0.121 + 0.013i & 0.204 + 0.059i & 0.432 - 0.013i & \frac{5}{9} \end{pmatrix}$$

$$\mathbf{P} = \mathbf{P}^\dagger$$

P isn't a projector because:  $\mathbf{P} \cdot \mathbf{P} \neq \mathbf{P}$

$$\mathbf{Q} = |a\rangle\langle b| = \begin{pmatrix} 0.116 + 0.116i \\ 0.233 + 0.164i \\ 0.349 + 0.465i \\ 0.465 + 0.581i \end{pmatrix} \cdot (0.365 + 0.073i \quad 0.438 - 0.073i \quad 0.51 - 0.126i \quad 0.583 + 0.219i)$$

$$\mathbf{Q} := \begin{pmatrix} 0.034 + 0.051i & 0.059 + 0.042i & 0.074 + 0.045i & 0.042 + 0.093i \\ 0.073 + 0.077i & 0.114 + 0.055i & 0.139 + 0.054i & 0.1 + 0.147i \\ 0.093 + 0.195i & 0.187 + 0.178i & 0.237 + 0.193i & 0.102 + 0.348i \\ 0.127 + 0.246i & 0.246 + 0.221i & 0.31 + 0.238i & 0.144 + 0.441i \end{pmatrix}$$

$$\mathbf{Q} \cdot \mathbf{Q} = \begin{pmatrix} -0.02 + 0.052i & -1.13 \times 10^{-4} + 0.066i & 5.893 \times 10^{-3} + 0.078i & -0.047 + 0.08i \\ -0.018 + 0.095i & 0.02 + 0.113i & 0.033 + 0.132i & -0.056 + 0.151i \\ -0.095 + 0.172i & -0.033 + 0.232i & -0.018 + 0.277i & -0.203 + 0.259i \\ -0.115 + 0.224i & -0.033 + 0.299i & -0.012 + 0.355i & -0.25 + 0.34i \end{pmatrix}$$

$\mathbf{Q} \cdot \mathbf{Q} \neq \mathbf{Q}$  Q isn't a projector

Example 6:

$$|a\rangle = \begin{pmatrix} 1 + j \\ 2 + j \cdot \sqrt{2} \\ 3 + j \cdot 4 \\ 4 + j \cdot 5 \end{pmatrix} \quad |b\rangle = \begin{pmatrix} -1 + i \\ -1.414 + 2i \\ -4 + 3i \\ -5 + 4i \end{pmatrix}$$

$$\langle b | = (-1 - i \quad -1.414 - 2i \quad -4 - 3i \quad -5 - 4i)$$

$$\mathbf{Q} = |a\rangle\langle b| = \begin{pmatrix} 1 + j \\ 2 + j \cdot \sqrt{2} \\ 3 + j \cdot 4 \\ 4 + j \cdot 5 \end{pmatrix} \cdot (-1 - i \quad -1.414 - 2i \quad -4 - 3i \quad -5 - 4i)$$

$$\mathbf{Q} := \begin{pmatrix} -2i & 0.586 - 3.414i & -1 - 7i & -1 - 9i \\ -0.586 - 3.414i & 4.271 \times 10^{-4} - 6i & -3.757 - 11.657i & -4.343 - 15.071i \\ 1 - 7i & 3.758 - 11.656i & -25i & 1 - 32i \\ 1 - 9i & 4.344 - 15.07i & -1 - 32i & -41i \end{pmatrix}$$

$$\mathbf{Q} \cdot \mathbf{Q} = \begin{pmatrix} -274.365 + 723.211i & -0.051 + 922.733i & 84.532 + 1.091i \times 10^3 & -648.475 + 1.122i \times 10^3 \\ -256.552 + 1.315i \times 10^3 & 270.159 + 1.575i \times 10^3 & 463.72 + 1.837i \times 10^3 & -778.33 + 2.106i \times 10^3 \\ -1.322 \times 10^3 + 2.394i \times 10^3 & -461.545 + 3.23i \times 10^3 & -249.45 + 3.859i \times 10^3 & -2.831 \times 10^3 + 3.604i \times 10^3 \\ -1.596 \times 10^3 + 3.117i \times 10^3 & -461.596 + 4.152i \times 10^3 & -164.918 + 4.95i \times 10^3 & -3.479 \times 10^3 + 4.726i \times 10^3 \end{pmatrix}$$

$\mathbf{h}$  is the set of the vectors  $\mathbf{P} \mathbf{x}$  with  $\mathbf{x} \in \mathbb{H}$  hence I can write

$$\mathbf{h} = \mathbf{P} \mathbb{H} \quad (10.4)$$

Let  $\mathbb{H} = \mathbb{R}^3$  that is the three dimensional euclidean space, and  $\mathbf{h}_a$  plane passing through the origin. Then  $\forall \mathbf{x} \in \mathbb{R}^3$ , let  $\mathbf{P}\mathbf{x}$  be the ordinary projection of  $\mathbf{x}$  onto the plane  $\mathbf{h}$ .

$$\mathbf{P}\mathbf{x} + (\mathbf{I} - \mathbf{P})\mathbf{x} = \mathbf{P}\mathbf{x} + \mathbf{x} - \mathbf{P}\mathbf{x} = \mathbf{x} \quad 10.5)$$

$$\mathbf{P}\mathbf{x} + (\mathbf{P} - \mathbf{I})\mathbf{x} = \mathbf{P}\mathbf{x} + \mathbf{P}\mathbf{x} - \mathbf{x} = \mathbf{x} \quad 10.6)$$

The projector  $\mathbf{I} - \mathbf{P}$  determines another subspace, the orthonormal one, denoted by  $\mathbf{h}^\perp$ . All vector  $|x_s\rangle$  of  $\mathbf{h}$  are orthonormal

to the vectors  $|x_n\rangle$  of  $\mathbf{h}^\perp$ . Then:

$$|x_s\rangle = \mathbf{P}|x\rangle$$

$$|x_n\rangle = (\mathbf{I} - \mathbf{P})|x\rangle$$

$$|x\rangle = \mathbf{P}|x\rangle + (\mathbf{I} - \mathbf{P})|x\rangle$$

verify the orthonormality:

$$\langle x_s | x_n \rangle = \langle x | \mathbf{P}(\mathbf{I} - \mathbf{P}) | x \rangle = \langle x | (\mathbf{P} - \mathbf{P}^2) | x \rangle = \langle x | (\mathbf{P} - \mathbf{P}) | x \rangle = 0$$

Two subspaces  $\mathbf{h}_1, \mathbf{h}_2 \subseteq \mathbb{H}$  are mutually orthogonal if  $\forall |x\rangle \in \mathbf{h}_1$  and if  $\forall |y\rangle \in \mathbf{h}_2$  results  $\langle x | y \rangle = 0$ .

The set  $\mathbf{h} = \{|x\rangle + |y\rangle : |x\rangle \in \mathbf{h}_1, |y\rangle \in \mathbf{h}_2\}$  is the *direct sum* of  $\mathbf{h}_1$  and  $\mathbf{h}_2$  and is denoted by:

$$\mathbf{h} = \mathbf{h}_1 \oplus \mathbf{h}_2. \quad 10.11)$$

For a collection of mutually orthogonal subspaces  $\mathbf{h}_1, \mathbf{h}_2, \dots, \mathbf{h}_n$  their direct sum is indicated so:

$$\mathbf{h} = \sum_j \oplus \mathbf{h}_j = \left\{ \sum_j |x_j\rangle : |x_j\rangle \in \mathbf{h}_j \right\}. \quad 10.12)$$

$\forall |x\rangle \in \mathbb{H}$  I can write  $|x\rangle = \mathbf{P}|x\rangle + (\mathbf{I} - \mathbf{P})|x\rangle$ , that is any projector  $\mathbf{P}$  gives a decomposition of  $\mathbb{H}$  into orthogonal spaces  $\mathbb{H} = \mathbf{h} \oplus (\mathbf{h}^\perp)$ . Furthermore  $\forall |x\rangle \in \mathbb{H}$ , the set  $\{\alpha | x\rangle : \alpha \in \mathbb{C}\}$  is a one dimensional subspace of  $\mathbb{H}$ , or the space spanned by  $|x\rangle$ . Given the basis  $\{|a_\gamma\rangle\} \in \mathbb{H}$ , the trace of the operator  $\mathbf{A}$  is:

$$\text{Tr}(\mathbf{A}) = \sum_\gamma \langle a_\gamma | \mathbf{A} | a_\gamma \rangle$$

10.13)

In effect the trace is independent from the basis.  $\text{Tr}(\mathbf{A} \cdot \mathbf{B}) = \text{Tr}(\mathbf{B} \cdot \mathbf{A})$

10.14)

$$\text{Tr}(\mathbf{A} + \mathbf{B}) = \text{Tr}(\mathbf{A}) + \text{Tr}(\mathbf{B}).$$

10.15)

Given  $|x_j\rangle \in \mathbf{h}_j$ , that is  $\mathbf{h}_j$  is the space spanned by  $|x_j\rangle$ , then the space  $\mathbb{H}$  is the *direct sum*:

$$\mathbb{H} = \sum_j \oplus \mathbf{h}_j = \mathbf{h}_0 \oplus \mathbf{h}_1 \oplus \mathbf{h}_2 \oplus \mathbf{h}_3 \oplus \dots \quad 10.16)$$

Let  $\mathbf{P}_n$ , with  $n=0,1,2,\dots$ , denote the projector on  $\mathbf{h}_n$ , then the operator form of the previous is:

$$\sum_{n=0}^{\infty} \mathbf{P}_n = \mathbf{I},$$

10.17)

so that  $\forall |f\rangle \in \mathbb{H}$ , I can write the sum of its components  $\mathbf{P}_n|f\rangle$  in the subspace  $\mathbf{h}_n$ , that is:

$$\text{which is equivalent writing: } |f\rangle |f\rangle = \sum_{n=0}^{\infty} (|a_n\rangle \langle a_n | f \rangle) \quad 10.18) \quad 10.19)$$

$$\text{Elementary projector } \mathbf{P}_a = |a\rangle \langle a| \quad 10.20)$$

$$\text{Tr}(|u\rangle \langle u|) = \langle u | u \rangle \quad 10.21)$$

$$\text{Tr}(|u\rangle \langle v|) = \langle v | u \rangle$$

$$|a\rangle \langle a| = \mathbf{I} \quad 10.22)$$

$$\text{Given the orthonormal set } \mathbf{h}^\perp = \{|k\rangle\} \text{ with } k=1,2,\dots,n, \text{ results: } \langle m | n \rangle = \delta_{m,n} \quad 10.23)$$

$$\text{the projector on the subset } E_1 \text{ is: } \mathbf{P}_1 = \sum_{j=1}^N |j\rangle \langle j| \quad 10.24)$$

$$\text{If given a ket } |\xi\rangle \text{ and } \xi \text{ is continuous in } (\xi_1, \xi_2), \text{ then } \langle \xi_1 | \xi \rangle = \Delta(\xi_1 - \xi) \quad 10.25)$$

$$\text{The projector on the subset } E_2 \text{ is: } \mathbf{P}_2 = \int_{\xi_1}^{\xi_2} |\xi\rangle d\xi \langle \xi| \quad 10.26)$$

$$\text{degenerate spectrum } \mathbf{P}_2 |u\rangle = \int_{\xi_1}^{\xi_2} |\xi\rangle d\xi \langle \xi | u \rangle \quad 10.27)$$

$$\text{Closure relation: } \mathbf{P}_A = \sum_{j=1}^N |j\rangle \langle j| + \int_{\xi_1}^{\xi_2} |\xi\rangle d\xi \langle \xi| = 1 \quad 10.28)$$

Expansion of any vector  $|\psi\rangle$  of Hilbert space in a series of the basic kets of the observable  $\mathbf{A}$ . I suppose that the spectrum of  $\mathbf{A}$  is non degenerate:

$$|\psi\rangle = \mathbf{P}_A |\psi\rangle = \sum_{k=1}^N |k\rangle \langle k | \psi \rangle + \int_{\xi_1}^{\xi_2} |\xi\rangle d\xi \langle \xi | \psi \rangle \quad 10.29)$$

$$\text{Parseval: } \langle \psi | \psi \rangle = \langle \psi | \mathbf{P}_A | \psi \rangle = \langle \psi | \left( \sum_{k=1}^N |k\rangle \langle k| + \int_{\xi_1}^{\xi_2} |\xi\rangle d\xi \langle \xi| \right) | \psi \rangle \quad 10.30)$$

$$\langle \psi | \psi \rangle = \sum_{k=1}^N (|\langle k | \psi \rangle|^2) + \int_{\nu_1}^{\nu_2} (|\langle \nu | \psi \rangle|^2) d\nu \quad 10.31)$$

$$\mathbf{H} = \mathbf{H} \mathbf{P}_H = \sum_{k=1}^N |k\rangle \lambda_k \langle k| + \int_{\nu_1}^{\nu_2} |\nu\rangle \lambda(\nu) d\nu \langle \nu| \quad 10.32)$$

$$f(\mathbf{H}) = \sum_{k=1}^N |k\rangle f(\lambda_k) \langle k| + \int_{\nu_1}^{\nu_2} |\nu\rangle f(\lambda(\nu)) d\nu \langle \nu| \quad (10.33)$$

**Example 1**

$$\mathbf{P}_i \leq \mathbf{P}_j \Rightarrow \mathbf{P}_i \cdot \mathbf{P}_j = \mathbf{P}_i \Rightarrow \langle u | \mathbf{P}_i | u \rangle \leq \langle u | \mathbf{P}_j | u \rangle \quad \forall |u\rangle \in \mathbb{H}$$

$$\mathbf{P}_1, \mathbf{P}_2, \dots, \mathbf{P}_n \quad \forall |u\rangle \in \mathbb{H} \Rightarrow \sum_{i=1}^n \langle u | \mathbf{P}_i | u \rangle = \langle u | u \rangle \Rightarrow \sum_{i=1}^n \mathbf{P}_i = \mathbf{P}$$

**Example 2**

$$(\nabla \times \nabla \times)^\dagger = \nabla \times \nabla \times \quad \text{I can write:}$$

$$\nabla \times \nabla \times \mathbf{E} = \lambda_n^2 \cdot \mathbf{E}$$

$$(\nabla \times \nabla \times) \mathbf{P}_H = \sum_{k=1}^N |k\rangle \lambda_k \langle k| + \int_{\nu_1}^{\nu_2} |\nu\rangle \lambda(\nu) d\nu \langle \nu|$$

Since the operator  $\nabla \times \nabla \times$  is *auto-adjoint or Hermitian*:  $\int_{\nu_1}^{\nu_2} |\nu\rangle \lambda(\nu) d\nu \langle \nu| = 0$

$$(\nabla \times \nabla \times) \mathbf{P}_H = \sum_{k=1}^N |k\rangle \lambda_k \langle k|$$

**II Commutator Operator [4]**

$$[ \mathbf{A}, \mathbf{B} ] = \mathbf{A} \cdot \mathbf{B} - \mathbf{B} \cdot \mathbf{A} \quad (11.1)$$

$$[ \mathbf{A}, \mathbf{B} ] = -[ \mathbf{B}, \mathbf{A} ] \quad (11.2)$$

$$[ \mathbf{A}, \text{Const} ] = \mathbf{A} \cdot \text{Const} - \text{Const} \cdot \mathbf{A} = 0 \quad (11.3)$$

$$[ \mathbf{A} + \mathbf{B}, \mathbf{C} ] = [ \mathbf{A}, \mathbf{C} ] + [ \mathbf{B}, \mathbf{C} ] \quad (11.4)$$

$$[ \mathbf{A}, \mathbf{B} \cdot \mathbf{C} ] = [ \mathbf{A}, \mathbf{B} ] \cdot \mathbf{C} + \mathbf{B} \cdot [ \mathbf{A}, \mathbf{C} ] \quad (11.5)$$

$$[ \mathbf{A} \cdot \mathbf{B}, \mathbf{C} ] = [ \mathbf{A}, \mathbf{C} ] \cdot \mathbf{B} + \mathbf{A} \cdot [ \mathbf{B}, \mathbf{C} ] \quad (11.6)$$

$$[ \mathbf{A} \mathbf{B}, \mathbf{C} \mathbf{D} ] = [ \mathbf{A}, \mathbf{C} ] \mathbf{D} \mathbf{B} + \mathbf{C} [ \mathbf{A}, \mathbf{D} ] \mathbf{B} + \mathbf{A} [ \mathbf{A}, \mathbf{C} ] \mathbf{D} + \mathbf{A} \mathbf{C} [ \mathbf{B}, \mathbf{D} ] \quad (11.7)$$

$$[ \mathbf{A} \cdot \mathbf{B}, \mathbf{C} \cdot \mathbf{D} ] = [ \mathbf{D}, \mathbf{C} ] \mathbf{B} \mathbf{D} + \mathbf{A} [ \mathbf{B}, \mathbf{C} ] \mathbf{D} + \mathbf{C} [ \mathbf{A}, \mathbf{D} ] \mathbf{B} + \mathbf{C} \mathbf{A} [ \mathbf{B}, \mathbf{D} ] \quad (11.8)$$

$$[ \mathbf{A}, [ \mathbf{B}, \mathbf{C} ] ] + [ \mathbf{B}, [ \mathbf{C}, \mathbf{A} ] ] + [ \mathbf{C}, [ \mathbf{A}, \mathbf{B} ] ] = 0 \quad (11.9)$$

$$[ \mathbf{A}, \mathbf{B}^n ] = \sum_{k=0}^{n-1} \mathbf{B}^k [ \mathbf{A}, \mathbf{B} ] \mathbf{B}^{n-k-1} \quad (10.10)$$

For a given quantum system in N dimensions. Position observables  $\mathbf{q}_i$   $i=1,2,\dots,N$

$$\text{Momentum observables } \mathbf{p}_i = -i \cdot \hbar \cdot \frac{\partial}{\partial \mathbf{q}_i}, i=1,2,\dots,N, \quad (10.11)$$

$$[ \mathbf{q}_i, \mathbf{q}_j ] = 0 \quad (10.12)$$

$$[ \mathbf{p}_i, \mathbf{p}_j ] = 0 \quad (10.13)$$

$$[ \mathbf{q}_i, \mathbf{p}_j ] = i \cdot \hbar \cdot \delta(i,j) \quad (10.14)$$

$$[ \mathbf{q}_i, \mathbf{F}(\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n) ] = 0 \quad (10.15)$$

$$[ \mathbf{p}_i, \mathbf{G}(\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_n) ] = 0 \quad (10.16)$$

$$[ \mathbf{p}_i, \mathbf{F}(\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n) ] = -i \cdot \hbar \cdot \frac{\partial}{\partial \mathbf{q}_i} \mathbf{F} \quad (10.17)$$

$$[ \mathbf{q}_i, \mathbf{G}(\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_n) ] = i \cdot \hbar \cdot \frac{\partial}{\partial \mathbf{p}_i} \mathbf{G} \quad (10.18)$$

$$[ \mathbf{p}_i, \mathbf{A}(\mathbf{p}_i, \mathbf{q}_i) ] = -i \cdot \hbar \cdot \frac{\partial}{\partial \mathbf{q}_i} \mathbf{A}(\mathbf{p}_i, \mathbf{q}_i) \quad (10.19)$$

$$\text{for a one-dimensional quantum system } [ \mathbf{q}, \mathbf{p}^n ] = i \cdot \hbar \cdot n \cdot \mathbf{p}^{n-1} \quad (10.20)$$

$$[ \mathbf{q}, \mathbf{p}^2 \cdot \mathbf{f}(\mathbf{q}) ] = 2i \cdot \hbar \cdot \mathbf{p} \cdot \mathbf{f}(\mathbf{q}) \quad (10.21)$$

$$[ \mathbf{q}, \mathbf{p} \cdot \mathbf{f}(\mathbf{q}) \cdot \mathbf{p} ] = i \cdot \hbar \cdot \mathbf{f}(\mathbf{q}) \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{f}(\mathbf{q}) \quad (10.22)$$

$$[ \mathbf{q}, \mathbf{f}(\mathbf{q}) \cdot \mathbf{p}^2 ] = 2i \cdot \hbar \cdot \mathbf{f}(\mathbf{q}) \cdot \mathbf{p} \quad (10.23)$$

$$[ \mathbf{p}, \mathbf{p}^2 \cdot f(\mathbf{q}) ] = -i \cdot \hbar \cdot \mathbf{p} \cdot \frac{\partial}{\partial \mathbf{q}} f(\mathbf{q}) \quad (10.24)$$

$$[ \mathbf{p}, \mathbf{p} \cdot f(\mathbf{q}) \cdot \mathbf{p} ] = -i \cdot \hbar \cdot \mathbf{p} \cdot \left( \frac{\partial}{\partial \mathbf{q}} f(\mathbf{q}) \right) \cdot \mathbf{p} \quad (10.25)$$

$$[ \mathbf{p}, f(\mathbf{q}) \cdot \mathbf{p}^2 ] = -i \cdot \hbar \cdot \left( \frac{\partial}{\partial \mathbf{q}} f(\mathbf{q}) \right) \cdot \mathbf{p}^2 \quad (10.26)$$

## 12 Operators' Algebra [4]

$$(\mathbf{A} \mathbf{B})^{-1} = \mathbf{B}^{-1} \mathbf{A}^{-1} \quad (12.1)$$

$$\langle v | = \langle u | \mathbf{A} \Rightarrow | v \rangle = \langle v |^* = (\langle u | \mathbf{A})^* = \mathbf{A}^\dagger | u \rangle \quad (12.2)$$

$$\langle y | \mathbf{A} | x \rangle = \langle x | \mathbf{A}^\dagger | y \rangle^* \quad (12.3)$$

$$(\mathbf{A}^\dagger)^\dagger = \mathbf{A} \quad (12.4)$$

$$(\text{const} \cdot \mathbf{A})^\dagger = \text{const}^* \cdot \mathbf{A}^\dagger \quad (12.5)$$

$$(\mathbf{A} + \mathbf{B})^\dagger = \mathbf{A}^\dagger + \mathbf{B}^\dagger \quad (12.6)$$

$$(\mathbf{A} \mathbf{B})^\dagger = \mathbf{B}^\dagger \mathbf{A}^\dagger \quad (12.7)$$

$$| u \rangle \langle v |^\dagger = | v \rangle \langle u | \quad (12.8)$$

$$\text{Hermitian or self-adjoint operator: } \mathbf{A} = \mathbf{A}^\dagger \Rightarrow \langle y | \mathbf{A} | x \rangle^* = \langle x | \mathbf{A} | y \rangle \quad (12.9)$$

$$\text{Anti - Hermitian operator } \mathbf{B} = -\mathbf{B}^\dagger \quad (12.10)$$

Each linear operator is formed by the sum of two operators, one Hermitian and the other anti - Hermitian:

$$\mathbf{A} = \mathbf{A} + \frac{\mathbf{A}^\dagger}{2} - \frac{\mathbf{A}^\dagger}{2} = \frac{\mathbf{A} + \mathbf{A}^\dagger}{2} + \frac{\mathbf{A} - \mathbf{A}^\dagger}{2} = \mathbf{A}_+ + \mathbf{A}_- \quad (12.11)$$

$$\mathbf{A}_+ = (\mathbf{A}_+)^\dagger \quad \mathbf{A}_- = -(\mathbf{A}_-)^\dagger$$

$$\text{Hermitian } \mathbf{A}_+ = \frac{\mathbf{A} + \mathbf{A}^\dagger}{2} \quad \mathbf{A}_- = \frac{\mathbf{A} - \mathbf{A}^\dagger}{2} \quad \text{anti - Hermitian} \quad (12.12)$$

$$\mathbf{C}_+ = \sum_{k=1}^n (\alpha_k \cdot \mathbf{A}_+) \quad (\forall \alpha_k \in \mathbb{R} \vee \mathbb{C}) \wedge \mathbf{A}_+ \in \mathbb{H} \Rightarrow \mathbf{C}_+ \in \mathbb{H} \quad (12.13)$$

$$\mathbf{A}_+ = (\mathbf{A}_+)^\dagger \quad \mathbf{B}_+ = (\mathbf{B}_+)^\dagger \Rightarrow (\mathbf{A}_+ \mathbf{B}_+)^\dagger = (\mathbf{B}_+)^\dagger (\mathbf{A}_+)^\dagger = \mathbf{B}_+ \mathbf{A}_+ = \mathbf{A}_+ \mathbf{B}_+ \quad (12.14)$$

The product of two Hermitian operators  $\mathbf{A}_+$  and  $\mathbf{B}_+$ , is Hermitian if and only if  $[\mathbf{A}_+, \mathbf{B}_+] = 0$ .

*The commutator of two Hermitian operators is anti - Hermitian:*

$$[\mathbf{C}_+, \mathbf{D}_+] = -([\mathbf{C}_+, \mathbf{D}_+])^\dagger \quad (12.15)$$

□ Demonstration of The commutator of two Hermitian operators is anti - Hermitian

$$\text{Operator's derivative } \frac{d}{d\xi} \mathbf{A}(\xi) = \lim_{\varepsilon \rightarrow 0} \frac{\mathbf{A}(\xi + \varepsilon) - \mathbf{A}(\xi)}{\varepsilon} \quad (12.16)$$

$$\text{Two operator's product derivative } \frac{d}{d\xi} (\mathbf{A} \mathbf{B}) = \left( \frac{d}{d\xi} \mathbf{A} \right) \cdot \mathbf{B} + \mathbf{A} \cdot \frac{d}{d\xi} \mathbf{B} \quad (12.17)$$

Operator's square derivative  $\frac{d}{d\xi} A^2 = \left(\frac{d}{d\xi} A\right) \cdot A + A \cdot \frac{d}{d\xi} A$  (12.18)

Operator's inverse derivative  $\frac{d}{d\xi} A^{-1} = -A^{-1} \cdot \left(\frac{d}{d\xi} A\right) \cdot A^{-1}$  (12.19)

Integral equation:  $B(t) = B_0 + i \cdot \left[ A, \int_0^t B(\tau) d\tau \right] \Rightarrow B(t) = e^{i \cdot A \cdot t} \cdot B_0 \cdot e^{-i \cdot A \cdot t}$  (12.20)

$$B(t) = B_0 + i \cdot \left[ A \cdot \int_0^t B(\tau) d\tau - \left( \int_0^t B(\tau) d\tau \right) \cdot A \right]$$

Definition:  $A(B)^k = [A, [A, [A, [A, [A, [A, [A, B]]]]]]$  k times (12.21)

$$e^{i \cdot A \cdot t} \cdot B \cdot e^{-i \cdot A \cdot t} = \sum_{k=0}^{\infty} \left( \frac{i^k}{k!} \cdot A(B)^k \right)$$
 (12.22)

$$A \left( \frac{d}{d\xi} A \right)^k = [A, [A, [A, [A, [A, [A, \frac{d}{d\xi} A]]]]]]$$
 (12.23)

$$e^{i \cdot A \cdot t} \cdot \frac{d}{d\xi} e^{-i \cdot A \cdot t} = i \cdot \sum_{k=0}^{\infty} \left[ \frac{(-i)^k}{(k+1)!} \cdot A \left( \frac{d}{d\xi} A \right)^k \right]$$
 (12.24)

### 13 Decomposition of the product of two Hermitian operators [4]

$$C_+ \cdot D_+ = \frac{C_+ \cdot D_+ + D_+ \cdot C_+}{2} + \frac{1}{2} \cdot ([C_+, D_+])$$
 (13.1)

Particular Hermitian Operator:  $|u\rangle \langle v|$  It has no inverse. (13.2)

$$|u\rangle \langle v| w\rangle = \text{const} \cdot (|u\rangle)$$
 (13.3)

$$\langle w| v\rangle \langle u| = \text{const} \cdot (\langle v|)$$
 (13.4)

### 14 Expectation value of the Operator

$$\langle A \rangle = \frac{\langle \psi | A | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int \Psi(\tau)^* \cdot A \cdot \Psi(\tau) d\tau}{\int \Psi(\tau)^* \cdot \Psi(\tau) d\tau}$$
 (14.1)

for normalized eigenfunction:  $\langle \psi | \psi \rangle = 1$

so that:  $\langle A \rangle = \langle \psi | A | \psi \rangle = \int \Psi(\tau)^* \cdot A \cdot \Psi(\tau) d\tau$  (14.2)

$$\langle F(A) \rangle = \sum_n P_n (\langle n | F(A) | n \rangle)$$
 (14.3)

$$\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle}$$
 (14.4)

$$\langle A - B \rangle = \langle \psi | A - B | \psi \rangle = \int \Psi(\tau)^* \cdot A \cdot \Psi(\tau) d\tau - \int \Psi(\tau)^* \cdot B \cdot \Psi(\tau) d\tau = \langle A \rangle - \langle B \rangle$$
 (14.5)

### 15 Heisenberg uncertainty principle

$$\Delta A \cdot \Delta B \geq \frac{1}{2} \cdot | \langle [A, B] \rangle |$$
 (15.1)

☐ Demonstration of 15.1)

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

$$A_1 = A - \langle A \rangle$$

$$\Delta A = \sqrt{\langle A_1^2 \rangle}$$

$$\Delta B = \sqrt{\langle (B - \langle B \rangle)^2 \rangle} = \sqrt{\langle B^2 \rangle - (\langle B \rangle)^2}$$

$$B_1 = B - \langle B \rangle$$

$$\Delta B = \sqrt{\langle B_1^2 \rangle}$$

$$(\Delta A \cdot \Delta B)^2 = (\langle A_1^2 \rangle) \cdot (\langle B_1^2 \rangle) = \langle \psi | A_1^2 | \psi \rangle \cdot \langle \psi | B_1^2 | \psi \rangle$$

*auto-adjoint or Hermitian operators:*

$$A_1 = A_1^\dagger \quad B_1 = B_1^\dagger$$

$$\langle \psi | A_1^2 | \psi \rangle \cdot \langle \psi | B_1^2 | \psi \rangle = \langle \psi | A_1 \cdot A_1 | \psi \rangle \cdot \langle \psi | B_1 \cdot B_1 | \psi \rangle$$

$$|z\rangle = A_1 | \psi \rangle \quad |\zeta\rangle = B_1 | \psi \rangle$$

$$\langle \psi | A_1 \cdot A_1 | \psi \rangle \cdot \langle \psi | B_1 \cdot B_1 | \psi \rangle = \langle \psi | A_1 | z \rangle \cdot \langle \psi | B_1 | \zeta \rangle$$

$$\langle \psi | A_1 | z \rangle = (\langle z | A_1 | \psi \rangle)^* = (\langle z | z \rangle)^* = (|A_1 | \psi \rangle)^2$$

$$\langle \psi | B_1 | \zeta \rangle = \langle \zeta | B_1 | \psi \rangle^* = (\langle \zeta | \zeta \rangle)^* = (|B_1 | \psi \rangle)^2$$

$$(\Delta A \cdot \Delta B)^2 = \langle \psi | A_1 | z \rangle \cdot \langle \psi | B_1 | \zeta \rangle = (|A_1 | \psi \rangle)^2 \cdot (|B_1 | \psi \rangle)^2$$

*Schwarz inequality:*

$$(|\langle x | A | y \rangle|)^2 \leq \langle x | A | x \rangle \cdot \langle y | A | y \rangle \quad (5.13')$$

$$(\Delta A \cdot \Delta B)^2 = (|A_1 | \psi \rangle)^2 \cdot (|B_1 | \psi \rangle)^2 = \langle \psi | A_1 | z \rangle \cdot \langle \psi | B_1 | \zeta \rangle \geq (|\langle \psi | A_1 \cdot B_1 | \psi \rangle|)^2$$

$$(\Delta A \cdot \Delta B)^2 \geq (|\langle \psi | A_1 \cdot B_1 | \psi \rangle|)^2$$

$$A_1 \cdot B_1 = \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} + \frac{A_1 \cdot B_1 - A_1 \cdot B_1}{2} = \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} + \frac{[A_1, B_1]}{2}$$

*auto-adjoint or Hermitian*

$$(A_1 \cdot B_1)^\dagger = (B_1)^\dagger \cdot (A_1)^\dagger = B_1 \cdot A_1$$

$$(\Delta A \cdot \Delta B)^2 \geq \left[ \left| \langle \psi | \left( \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} + \frac{[A_1, B_1]}{2} \right) | \psi \rangle \right|^2 \right]$$

$$(\Delta A \cdot \Delta B)^2 \geq \left( \left| \langle \psi | \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} | \psi \rangle + \langle \psi | \frac{[A_1, B_1]}{2} | \psi \rangle \right|^2 \right)$$

$$\langle \psi | \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} | \psi \rangle = \left\langle \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} \right\rangle$$

$$\langle \psi | \frac{[A_1, B_1]}{2} | \psi \rangle = \left\langle \frac{[A_1, B_1]}{2} \right\rangle$$

$$(\Delta A \cdot \Delta B)^2 \geq \left( \left| \left\langle \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} \right\rangle + \left\langle \frac{[A_1, B_1]}{2} \right\rangle \right|^2 \right)$$

assuming that the average  $\left\langle \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} \right\rangle$  is real and  $\left\langle \frac{[A_1, B_1]}{2} \right\rangle$  is imaginary, I get:

$$\left\langle \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} \right\rangle = \langle \psi | \frac{A_1 \cdot B_1}{2} | \psi \rangle + \langle \psi | \frac{B_1 \cdot A_1}{2} | \psi \rangle$$

$$A_1 = \alpha \cdot B_1$$

$$\langle \psi | \frac{A_1 \cdot B_1}{2} | \psi \rangle + \langle \psi | \frac{B_1 \cdot A_1}{2} | \psi \rangle = (\alpha^* + \alpha) \cdot \langle \psi | \frac{B_1 \cdot B_1}{2} | \psi \rangle = \text{Re}(\alpha) \cdot \langle \psi | \frac{B_1^2}{2} | \psi \rangle$$

$$\boxed{\text{Re}(\alpha) \cdot \langle \psi | \frac{B_1^2}{2} | \psi \rangle = 0} \quad \text{if } \text{Re}(\alpha) = 0$$

$$(\Delta A \cdot \Delta B)^2 \geq \left( \left| \left\langle \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} \right\rangle \right|^2 + \left( \left| \left\langle \frac{[A_1, B_1]}{2} \right\rangle \right|^2 \right) \right)$$

The minimum for  $\Delta A \cdot \Delta B$  is reached when  $\langle A_1 \cdot B_1 + B_1 \cdot A_1 \rangle = 0$  finally resulting:

$$(\Delta A \cdot \Delta B)^2 \geq \left( \left| \left\langle \frac{[A_1, B_1]}{2} \right\rangle \right|^2 \right)$$

$$A_1 = A - \langle A \rangle$$

$$B_1 = B - \langle B \rangle$$

$$[A_1, B_1] = A_1 \cdot B_1 - B_1 \cdot A_1 = (A - \langle A \rangle) \cdot (B - \langle B \rangle) - (B - \langle B \rangle) \cdot (A - \langle A \rangle)$$

$$\left[ \begin{aligned} &(A - \langle A \rangle) \cdot (B - \langle B \rangle) \dots \\ &+ [((B - \langle B \rangle) \cdot (A - \langle A \rangle))] \end{aligned} \right] = A \cdot B - A \langle B \rangle - \langle A \rangle B + \langle A \rangle \langle B \rangle \dots$$

$$+ (-B \cdot A + B \langle A \rangle + \langle B \rangle A - \langle A \rangle \langle B \rangle)$$

$$A \cdot B - A \langle B \rangle - \langle A \rangle B + \langle A \rangle \langle B \rangle - B \cdot A + B \langle A \rangle + \langle B \rangle A - \langle B \rangle \langle A \rangle$$

$$A \langle B \rangle = \langle B \rangle A$$

$$\langle A \rangle B = B \langle A \rangle$$

$$\langle A \rangle \langle B \rangle = \langle B \rangle \langle A \rangle$$

$$[A_1, B_1] = A \cdot B - B \cdot A$$

$$\Delta A \cdot \Delta B \geq \frac{1}{2} \cdot |\langle [A_1, B_1] \rangle| = \frac{1}{2} \cdot |\langle [A, B] \rangle|$$

$$\boxed{\Delta A \cdot \Delta B \geq \frac{1}{2} \cdot |\langle [A, B] \rangle|}$$

□ Demonstration of 15.1)

Each physical system possesses its dynamical variables, each one at each instant possessing a well defined value. The set of all those values defines the dynamical state of the system at that instant.

Consider an elementary particle of mass  $m_p$  and kinetic energy  $T_p = \frac{p^2}{2 \cdot m_p}$ . Then I can write  $p = \sqrt{2 \cdot m_p \cdot T_p}$  and since

$$p = \hbar \cdot k_p, \text{ where } k_p = \frac{2 \cdot \pi}{\lambda_p}, \text{ results the wavelength of the particle } \lambda_p = \frac{2 \cdot \pi \cdot \hbar}{\sqrt{2 \cdot m_p \cdot T_p}} = \frac{h}{\sqrt{2 \cdot m_p \cdot T_p}} \text{ which is the known de}$$

Brogie wavelength of the particle. For example if  $m_p := m_e$  and  $T_{p1} := 1 \cdot eV$ , the de Broglie wavelength is

$$\lambda_e := \frac{h}{\sqrt{2 \cdot m_p \cdot T_{p1}}} = 12.27 \cdot \text{\AA} \text{ so that if } T_p = z_p \cdot T_{p1} \text{ with } z_p := 5 \cdot 10^4 \text{ then } \lambda_p := \frac{12.265 \text{\AA}}{\sqrt{z_p}} \text{ that is } \lambda_p = 0.05 \cdot \text{\AA}$$

Consider a monochromatic plane wave associated with a particle which propagates in an isotropic and homogeneous medium:

$$E(\mathbf{r}, t) = E_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega \cdot t)}, \quad (16.1)$$

where the wavelength is  $\lambda = \frac{2 \cdot \pi}{|\mathbf{k}|}$  and  $\mathbf{k} \cdot \mathbf{r} - \omega \cdot t = \text{constant}$  The time derivative of the latter gives:

$$\frac{\partial}{\partial t} (\mathbf{k} \cdot \mathbf{r} - \omega \cdot t) = \mathbf{k} \cdot \frac{\partial \mathbf{r}}{\partial t} - \omega = 0, \text{ that is the phase velocity } \left| \frac{\partial \mathbf{r}}{\partial t} \right| = \frac{\omega}{|\mathbf{k}|} = v_\varphi \quad (16.2)$$

Each wave can be considered as a superposition of monochromatic plane waves. The dispersion law  $\omega(k)$ , let me know the time behavior of every wave. To each frequency corresponds an energy  $E_1 = \hbar \cdot \omega_1$

The classical approximation let me found a relation between  $\mathbf{k}$  and the moment  $\mathbf{p}$  of the particle.

Indeed to the particle is associated the wave packet:

$$\Psi(\mathbf{r}, t) = \int_{-\infty}^{\infty} f_{pw}(k_1) \cdot e^{i(\mathbf{k}_1 \cdot \mathbf{r} - \omega_1 \cdot t)} dk_1, \quad (16.3)$$

where  $f_{pw}(k_1) = A(k_1) \cdot e^{i\alpha(k_1)}$  is the plane wave spectrum and  $A(k_1)$  takes appreciable values only around  $k_1$ .

In one dimension I get:

$$\Psi(x, t) = \int_{-\infty}^{\infty} f_{pw}(k_1) \cdot e^{i(k_1 \cdot x - \omega_1 \cdot t)} dk_1 = \int_{-\infty}^{\infty} A(k_1) \cdot e^{i\varphi(k_1)} dk_1, \quad (16.4)$$

where  $\varphi(k_1) = k_1 \cdot x - \omega_1 \cdot t + \alpha(k_1)$ . The function  $A(k_1)$  has a pick in a region  $\Delta k$  around  $k_1$ . The wave is

concentrated in a region  $\Delta x \approx \left( \frac{1}{\Delta k_1} \right)$ , where  $\frac{\partial}{\partial k_1} \varphi(k_1) = x - t \cdot \frac{\partial}{\partial k_1} \omega(k_1) + \frac{\partial}{\partial k_1} \alpha(k_1) = 0$ , namely

(16.5)

$$x = t \cdot \frac{\partial}{\partial k_1} \omega(k_1) - \frac{\partial}{\partial k_1} \alpha(k_1), \quad (16.6)$$

with a velocity:

$$\frac{\partial x}{\partial t} = v_g = \frac{\partial}{\partial k_1} \omega(k_1). \quad (16.7)$$

For the classical approximation where the extension of the wave packet is traceable, the particle velocity is

$$v = \frac{\partial}{\partial p} E = v_g = \frac{\partial}{\partial k_1} \omega(k_1), \quad (16.8)$$

$$\text{that is } \frac{\partial}{\partial p} E = \frac{\partial}{\partial k_1} \omega(k_1). \quad (16.9)$$

$$\text{Multiplying and dividing the right side by } \hbar, \text{ I get: } \frac{\partial}{\partial p} E = \frac{1}{\hbar} \cdot \frac{\partial}{\partial k_1} (\omega(k_1) \cdot \hbar), \quad (16.10)$$

$$\text{from which I have: } E = \hbar \cdot \omega \text{ and } p = \hbar \cdot k_1. \quad (16.11)$$

### Postulates

Then the wave function of the quantum system define completely its dynamical state. It is the equation of the wave propagation:

$$\Psi(\mathbf{r}, t) = \int_{-\infty}^{\infty} \psi(\mathbf{p}) \cdot e^{i\left(\frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar}\right)} d\mathbf{p}, \quad (16.12)$$

$$\text{which is rewritten as: } \Psi(\mathbf{r}, t) = A_\psi \cdot e^{-i \cdot \frac{E \cdot t}{\hbar}}. \quad (16.13)$$

This is a solution of the differential equation:

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = E \cdot \Psi(\mathbf{r}, t), \quad (16.14)$$

$$\text{in fact: } i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = E \cdot A_\psi \cdot e^{-\frac{E \cdot t \cdot i}{\hbar}} \quad (16.15)$$

$$E \cdot A_\psi \cdot e^{-\frac{E \cdot t \cdot i}{\hbar}} = E \cdot \Psi(\mathbf{r}, t) = E \cdot A_\psi \cdot e^{-i \cdot \frac{E \cdot t}{\hbar}}. \quad (16.16)$$

The classical kinetic energy is:  $E = \frac{p^2}{2 \cdot m}$

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = E \cdot \Psi(\mathbf{r}, t) = \int_{-\infty}^{\infty} E \cdot \psi(\mathbf{p}) \cdot e^{i\left(\frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar}\right)} d\mathbf{p}, \quad (16.17)$$

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \frac{1}{2 \cdot m} \cdot \int_{-\infty}^{\infty} \mathbf{p}^2 \cdot \psi(\mathbf{p}) \cdot e^{i\left(\frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar}\right)} d\mathbf{p}, \quad (16.18)$$

$$\nabla \Psi(\mathbf{r}, t) = \nabla \int_{-\infty}^{\infty} \psi(\mathbf{p}) \cdot e^{i\left(\frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar}\right)} d\mathbf{p} = \frac{i}{r} \cdot \int_{-\infty}^{\infty} \mathbf{p} \cdot \psi(\mathbf{p}) \cdot e^{i\left(\frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar}\right)} d\mathbf{p} \quad (16.19)$$

$$\int_{-\infty}^{\infty} \mathbf{p} \cdot \psi(\mathbf{p}) \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} \quad (16.20)$$

$$-\hbar^2 \cdot \Delta \Psi(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{p}^2 \cdot \psi(\mathbf{p}) \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} = 2 \cdot m \cdot i \cdot \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) \quad (16.21)$$

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \frac{-\hbar^2}{2 \cdot m} \cdot \Delta \Psi(\mathbf{r}, t) \quad (16.22)$$

☑ Schrödinger equation ([4] Vol. I)

The theory of matter waves leads unambiguously to the wave equation of a free particle (non relativistic approximation). The

wave  $\Psi(\mathbf{r}, t)$  is a superposition of monochromatic waves  $e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)}$ :

$$\Psi(\mathbf{r}, t) = \int \Theta(\mathbf{p}) \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} \quad (16.23)$$

where

$$\mathbf{p} = p_x \cdot \mathbf{i}_x + p_y \cdot \mathbf{i}_y + p_z \cdot \mathbf{i}_z \quad \mathbf{r} = x \cdot \mathbf{i}_x + y \cdot \mathbf{i}_y + z \cdot \mathbf{i}_z \quad (16.24)$$

with angular frequency  $\omega = \frac{E}{\hbar}$  connected to the wave vector  $\mathbf{k} = \frac{\mathbf{p}}{\hbar}$  by the relation connecting momentum and energy

$E = \frac{\mathbf{p}^2}{2 \cdot m}$ . Taking the partial derivative equation of 1) one obtains:

$$\frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \int \Theta(\mathbf{p}) \cdot \frac{\partial}{\partial t} e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} = \frac{-i}{\hbar} \int \Theta(\mathbf{p}) \cdot E \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} \quad (16.25)$$

$$\text{that is } \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \frac{-i}{\hbar} \int \Theta(\mathbf{p}) \cdot E \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p}$$

$$\text{or also } i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \int \Theta(\mathbf{p}) \cdot E \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} \quad (16.26)$$

Now calculate the gradient of 16.23):

$$\nabla \Psi(\mathbf{r}, t) = \nabla \int \Theta(\mathbf{p}) \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} = \int \Theta(\mathbf{p}) \cdot \nabla e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} \quad (16.27)$$

$$\text{that is } \nabla e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} = \frac{i}{\hbar} \cdot \mathbf{p} \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} \quad (16.28)$$

$$\nabla \Psi(\mathbf{r}, t) = \frac{i}{\hbar} \int \Theta(\mathbf{p}) \cdot \mathbf{p} \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} \quad (16.29)$$

Then the divergence of it:

$$\nabla \cdot \nabla \Psi(\mathbf{r}, t) = \Delta \Psi(\mathbf{r}, t) = \frac{i}{\hbar} \cdot \nabla \cdot \int \Theta(\mathbf{p}) \cdot \mathbf{p} \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} = \frac{i}{\hbar} \int \Theta(\mathbf{p}) \cdot \mathbf{p} \cdot \nabla \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p}$$

$$\Delta \Psi(\mathbf{r}, t) = \frac{1}{\hbar^2} \int \Theta(\mathbf{p}) \cdot \mathbf{p}^2 \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} \quad (16.30)$$

since  $\mathbf{p}^2 = 2 \cdot m \cdot E$ , after a substitution one gets:

$$\frac{-\hbar^2}{2 \cdot m} \cdot \Delta \Psi(\mathbf{r}, t) = \int \Theta(\mathbf{p}) \cdot E \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} \quad (16.31)$$

The right side of 16.31) is the same of eq 16.26) below rewritten

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \int \Theta(\mathbf{p}) \cdot E \cdot e^{i \left( \frac{\mathbf{p} \cdot \mathbf{r} - E \cdot t}{\hbar} \right)} d\mathbf{p} \quad (16.26)$$

equating 16.26) and eq 16.31) I get:

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \frac{-\hbar^2}{2 \cdot m} \cdot \Delta \Psi(\mathbf{r}, t)$$

this is the well known three dimensional Schrödinger equation for a free particle of mass m.

**Laplace transform of the Schrödinger equation :**

$$|\Psi(x, s)\rangle = \mathcal{L}(|\psi(x, t)\rangle) \quad i \cdot \hbar \cdot [s \cdot (|\Psi(z, s)\rangle) - |\psi(0)\rangle] = \mathbf{H} |\Psi(z, s)\rangle \quad (16.32)$$

Furthermore the equation can be deduced from a **system of two partial differential equation:**

$$\frac{\partial}{\partial z} \Psi(z, t) = j \cdot \varphi(z, t) \quad \frac{\partial}{\partial z} \varphi(z, t) = \frac{2 \cdot m}{\hbar} \cdot \frac{\partial}{\partial t} \Psi(z, t) - j \cdot \frac{2 \cdot m \cdot V(z)}{\hbar} \cdot \Psi(z, t)$$

☑ Schrödinger equation ([4] Vol. I)



### 17 Correspondence Principle. Quantization procedures

when the quantum system possesses a classical analogue

Quantization rules (substitute to each classical operator of the Hamiltonian the corresponding Quantum Operator)

Classical Operator	Quantum Operator acting on kets or eigenfunctions	
$\mathbf{p}$	$\leftrightarrow -i\hbar \cdot \nabla$	(17.1)

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \leftrightarrow -i\hbar \cdot \mathbf{r} \times \nabla, \quad (17.2)$$

$$\mathbf{s} \cdot \mathbf{p} \leftrightarrow \nabla \times \quad [4] \ 551$$

$$\mathbf{p}^2 \leftrightarrow -\hbar^2 \cdot \Delta, \quad (17.3)$$

$$\frac{\mathbf{p} \cdot \mathbf{q}'}{2} = \frac{\mathbf{p}^2}{2 \cdot m} \leftrightarrow \frac{-\hbar^2}{2 \cdot m} \cdot \Delta \quad (17.4)$$

$$\text{Energy } E \leftrightarrow i\hbar \cdot \frac{\partial}{\partial t}, \quad (17.5)$$

$$E^2 \leftrightarrow -\hbar^2 \cdot \frac{\partial^2}{\partial t^2}$$

$$\mathbf{r}^2 = (\mathbf{r} \times \mathbf{p}) \cdot (\mathbf{r} \times \mathbf{p}) = r^2 \cdot (\mathbf{p}^2 - p_r^2) \leftrightarrow r^2 \cdot \left[ -\hbar^2 \cdot \Delta + \hbar^2 \cdot \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \right] \text{Sph. coord.} \quad (17.6)$$

$$\mathbf{r} \cdot \mathbf{p} \leftrightarrow -i\hbar \cdot \mathbf{r} \cdot \frac{\partial}{\partial \mathbf{r}} = -i\hbar \cdot \mathbf{r} \cdot \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \text{Sph. coord.} \quad (17.7)$$

$$\mathbf{A} \text{ is the vector potential } \mathbf{p} \cdot \mathbf{A} \leftrightarrow \frac{i\hbar}{2} \cdot (\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla). \quad (17.8)$$

**Example 17.1) Heisenberg Uncertainty principle for two linear Operators A and B:**

$$\Delta \mathbf{A} \cdot \Delta \mathbf{B} \geq \frac{1}{2} \cdot | \langle [ \mathbf{A}, \mathbf{B} ] \rangle |$$

For a particle of mass m

$$\mathbf{x} = \mathbf{q} \quad \mathbf{q} \leftrightarrow \mathbf{q} = \mathbf{A} \quad \mathbf{p} = m \cdot \mathbf{v} \quad \mathbf{p} \leftrightarrow \left( \frac{\hbar}{i} \cdot \nabla = \mathbf{B} \right) \quad \mathbf{i} = i$$

$$[ \mathbf{A}, \mathbf{B} ] \Psi = \left[ \mathbf{x}, \frac{\hbar}{i} \cdot \nabla \right] \Psi = \mathbf{x} \cdot \frac{\hbar}{i} \cdot \nabla \Psi - \frac{\hbar}{i} \cdot \nabla \mathbf{x} \cdot \Psi = \mathbf{x} \cdot \frac{\hbar}{i} \cdot \nabla \Psi - \frac{\hbar}{i} \cdot \nabla \mathbf{x} \cdot \Psi - \frac{\hbar}{i} \cdot \mathbf{x} \cdot \nabla \Psi = -\frac{\hbar}{i} \cdot \Psi \cdot \nabla \mathbf{x} = -\frac{\hbar}{i} \cdot \Psi$$

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

$$\Delta \mathbf{A} \cdot \Delta \mathbf{B} = \Delta \mathbf{x} \cdot \Delta \mathbf{p} \geq \frac{1}{2} \cdot |i\hbar| = \frac{1}{2} \cdot \hbar$$

$$\Delta \mathbf{x} \cdot \Delta \mathbf{p} \geq \frac{1}{2} \cdot \hbar \quad (17.9)$$

"A similar trade-off occurs when attempting to measure the energy of a quantum system at a given time. An instantaneous measurement implies a high-frequency probe, but this means a high-energy probe which will mask the energy of the quantum state itself. Conversely, a very low energy probe, which will unduly affect the energy of the quantum state, implies a low-frequency probe, which means the time to be associated with the measurement is uncertain, thus:

$$\Delta t \cdot \Delta E \geq \hbar \quad [11]$$

□

**Example 17.3) Relativistic case:**  $E = \pm c \cdot \sqrt{\mathbf{p}^2 + m_p^2 \cdot c^2} \quad (17.10)$

$$E^2 = c^2 \cdot \mathbf{p}^2 + m_p^2 \cdot c^4 \quad (17.11)$$

applying the correspondence principle I get:

$$-\hbar^2 \cdot \frac{\partial^2}{\partial t^2} \Psi = -c^2 \cdot \hbar^2 \cdot \Delta \Psi + m_p^2 \cdot c^4 \cdot \Psi \quad (17.12)$$

divide by  $c^2 \cdot \hbar^2$

$$\Delta \Psi - \frac{1}{c^2} \cdot \frac{\partial^2}{\partial t^2} \Psi - \frac{m_p^2 \cdot c^2}{\hbar^2} \cdot \Psi = 0 \quad (17.13)$$

or using the **Dalambertian Operator:**  $\square = \left( \frac{1}{c} \right)^2 \cdot \frac{\partial^2}{\partial t^2} - \nabla^2, \quad (17.15)$

**Relativistic free particle Klein-Gordon equation:**  $\square + \left( \frac{m_p \cdot c}{\hbar} \right)^2 \Psi(\mathbf{r}, t) = 0 \quad (17.16)$

□

$$\frac{\partial^2}{\partial x^2} \Psi + \frac{\partial^2}{\partial y^2} \Psi + \frac{\partial^2}{\partial z^2} \Psi = \left( \sum_{\mu=1}^3 \partial_{\mu}^2 \right) \Psi = \partial_{\mu}^2 \Psi \quad (17.17)$$

$$\partial_x^2 + \partial_y^2 + \partial_z^2 = \sum_{\mu=1}^3 \partial_{\mu}^2 \quad \partial_{\mu}^2 \quad (17.18)$$

$$p_{\mu} = i \cdot \partial_{\mu} \quad (17.19)$$

$$\square = \partial_{\mu} \cdot \partial^{\mu} = \frac{1}{c^2} \cdot \partial_t^2 - \nabla^2 = -p^2 \quad (17.20)$$

□ Analytical solution for relativistic free particle

## 18 Lagrange equations

Lagrangian coordinates for a system with n degree of freedom :  $q_i, i=1,..n$

Kinetic energy : T

Potential energy : U

Classical mechanics Lagrangian :

$$L(q_1, q_2, \dots, q_n, q'_1, q'_2, \dots, q'_n, t) = T(q'_1, q'_2, \dots, q'_n, t) - U(q_1, q_2, \dots, q_n) \quad (18.1)$$

Lagrange equations' system

$$\frac{d}{dt} \frac{\partial L}{\partial q'_i} - \frac{\partial L}{\partial q_i} = 0 \quad i = 1, 2, 3 \dots n \quad (18.2)$$

Conjugated momenta  $p_i = \frac{\partial L}{\partial q'_i} \quad i = 1, 2, 3 \dots n$  Kinetic energy:  $T = \frac{1}{2 \cdot m_p} \cdot \sum_{i=1}^n p_i^2 = \frac{1}{2 \cdot m_p} \cdot \sum_{i=1}^n \left( \frac{\partial L}{\partial q'_i} \right)^2$

$$T_i = \frac{p_i^2}{2 \cdot m_p} = \frac{p_i \cdot p_i}{2 \cdot m_p} = \frac{p_i \cdot m_p \cdot q'_i}{2 \cdot m_p} = \frac{p_i \cdot q'_i}{2} \Rightarrow T = \frac{1}{2} \cdot \sum_{i=1}^n (p_i \cdot q'_i)$$

$$\Rightarrow L = \frac{1}{2} \cdot \sum_{i=1}^n (p_i \cdot q'_i) - U \quad (18.3)$$

Example: Lagrange equations for a classical two degree of freedom System

## 19 Hamilton equations

Kinetic energy : T, Potential energy : U

Classical mechanics Hamiltonian :

$$H(q_1, q_2, \dots, q_n, p_1, p_2, \dots, p_n, t) = T + U = 2 \cdot T - L(q_1, q_2, \dots, q_n, q'_1, q'_2, \dots, q'_n, t) = E$$

$$H = 2 \cdot T - L = 2 \cdot \frac{1}{2} \cdot \sum_{i=1}^n (p_i \cdot q'_i) - L = \sum_{i=1}^n (p_i \cdot q'_i) - L = \sum_{i=1}^n \left( q'_i \cdot \frac{\partial L}{\partial q'_i} \right) - L = E$$

$$E = H = \sum_{i=1}^n \left( q'_i \cdot \frac{\partial L}{\partial q'_i} \right) - L \quad (19.1)$$

$$q'_i = \frac{\partial H}{\partial p_i} \quad i = 1, 2, 3 \dots n \quad (19.2)$$

$$p'_i = - \frac{\partial H}{\partial q_i} \quad (19.3)$$

Solution of the one-dimensional Schrödinger equation for a free particle[1]

Standing wave

Infinitely high potential barrier

Classical Hamiltonian for N non relativistic particles of rest mass  $m_i$ , under mutual interaction only

Classical Hamiltonian for two non relativistic particles of rest mass  $m_1$  and  $m_2$ , under mutual interaction only

Classical Hamiltonian for two non relativistic and non interacting particles of rest mass  $m_1$  and  $m_2$

Potential hole between two walls

Scattering on a Dirac Delta Barrier

Finite Potential Barrier. Resonances

Potential Step. Reflection and Transmission of Wave

Scattering on a Symmetrical Potential Barrier. Tunnel Effect

Reflexion Inversion

Rectangular Potential Hole - Bound State

Rectangular Hole Between Walls

Virtual Levels

Periodic Potential's Wave Function

Potential Formed By A Sequence of Dirac Pulses Spaced  $\Delta$  From Each Other

Numerical solution of a one dimensional Schrödinger equation

## 20 Schrödinger equation of motion

System's time evolution. Given a physical system whose Hamiltonian (observable) is known, and are given the initial conditions the equations are the following:

$$i\hbar \cdot \frac{\partial}{\partial t} |\psi\rangle = \mathbf{H} |\psi\rangle \quad (20.1)$$

$$-i\hbar \cdot \frac{\partial}{\partial t} \langle \psi | = \langle \psi | \mathbf{H}^\dagger \quad (20.2)$$

They are deterministic.

A **system is conservative if the Hamiltonian isn't time dependent** otherwise isn't conservative. Each isolated system is conservative.

Assuming  $\mathbf{H}(t) = \mathbf{H}$  time independent and with a discrete spectrum only, I can create the following base system belonging to the Hilbert space:

$$\mathbf{H} |k\rangle = E_k |k\rangle, \quad (20.3)$$

from the closure relation I know that  $\mathbf{P}_n = \sum_{k=1}^N |k\rangle \langle k| + \int_{\xi_1}^{\xi_2} |\xi\rangle d\xi \langle \xi| = 1$ , (20.4)

since there exist only the discrete spectrum for hypothesis, the integral vanishes, so that:

$$\mathbf{P}_n = \sum_{k=1}^N |k\rangle \langle k| = 1 \quad (20.5)$$

and the equation 20.1) become:  $i\hbar \cdot \sum_{k=1}^N |k\rangle \langle k| \frac{\partial}{\partial t} |\psi\rangle = \sum_{k=1}^N |k\rangle \langle k| \mathbf{H} |\psi\rangle$ , (20.6)

since  $|k\rangle$  is time independent, I can write:

$$i\hbar \cdot \sum_{k=1}^N |k\rangle \frac{\partial}{\partial t} \langle k | \psi \rangle = \sum_{k=1}^N |k\rangle \langle k | \mathbf{H} | \psi \rangle \quad (20.7)$$

furthermore, since  $\mathbf{H} | \psi \rangle = E_k | \psi \rangle$  substituting in (20.7), I get:

$$i\hbar \cdot \sum_{k=1}^N |k\rangle \frac{\partial}{\partial t} \langle k | \psi \rangle = \sum_{k=1}^N |k\rangle \langle k | E_k | \psi \rangle \quad (20.8)$$

$$i\hbar \cdot \sum_{k=1}^N |k\rangle \frac{\partial}{\partial t} \langle k | \psi \rangle - \sum_{k=1}^N |k\rangle \langle k | E_k | \psi \rangle = 0 \quad (20.9)$$

$$\sum_{k=1}^N \left( i\hbar \cdot |k\rangle \frac{\partial}{\partial t} \langle k | \psi \rangle - |k\rangle E_k \langle k | \psi \rangle \right) = 0 \quad (20.10)$$

$$\sum_{k=1}^N |k\rangle \left( i\hbar \cdot \frac{\partial}{\partial t} \langle k | \psi \rangle - E_k \langle k | \psi \rangle \right) = 0 \quad (20.11)$$

All the components must vanish otherwise the basis isn't complete:

$$i\hbar \cdot \frac{\partial}{\partial t} \langle k | \psi \rangle - E_k \langle k | \psi \rangle = 0 \quad (20.12)$$

the solution is:  $\langle k | \psi \rangle = C \cdot e^{-i \cdot \frac{E_k}{\hbar} \cdot t}$  (20.13)

and the initial condition let me know the constant C:

for  $t = t_0$ , I get:  $C = \left( \langle k | \psi_0 \rangle \right) \cdot e^{i \cdot \frac{E_k}{\hbar} \cdot t_0} \Rightarrow \langle k | \psi \rangle = \langle k | \psi_0 \rangle \cdot e^{-i \cdot \frac{E_k}{\hbar} \cdot (t-t_0)}$  (20.14)

$$|k\rangle \langle k | \psi \rangle = |k\rangle \langle k | \psi_0 \rangle \cdot e^{-i \cdot \frac{E_k}{\hbar} \cdot (t-t_0)} \quad (20.15)$$

$$|k\rangle \langle k | = 1 \quad | \psi \rangle = | \psi_0 \rangle \cdot e^{-i \cdot \frac{E_k}{\hbar} \cdot (t-t_0)} \quad (20.16)$$

$$f(\mathbf{H}) |k\rangle = f(E_k) |k\rangle \quad (20.17)$$

$$f(\mathbf{H}) = \sum_{k=1}^N |k\rangle f(E_k) \langle k| = \sum_{k=1}^N |k\rangle e^{-i \cdot \frac{E_k}{\hbar} \cdot (t-t_0)} \langle k| = \sum_{k=1}^N |k\rangle e^{-i \cdot \frac{\mathbf{H}}{\hbar} \cdot (t-t_0)} \langle k| \quad (20.18)$$

$$| \psi \rangle = e^{-i \cdot \frac{\mathbf{H}}{\hbar} \cdot (t-t_0)} | \psi_0 \rangle \quad (20.19)$$

$U(t) = e^{-i \cdot \frac{\mathbf{H}}{\hbar} \cdot (t-t_0)}$  is the **evolution operator**. It is unitary. The ket  $| \psi \rangle$  components, are those of  $| \psi_0 \rangle$  rotated with a phase

$$\frac{E_k}{\hbar} = \omega_k \quad (20.20)$$

**Planck's formula:**  $E(\omega_k) := \hbar \cdot \omega_k$  (20.21)

## 21 Black body radiation

The *spectral exitance* is given by the Planck formula.

Define the constants.  $c_1 := \pi \cdot 2 \cdot h \cdot c^2$        $c_2 := \frac{h \cdot c}{k_B}$

$c_1 = 0.32 \cdot \frac{\text{cal} \cdot \mu\text{m}^2}{\text{hr}}$        $c_2 = 0.01 \text{ m} \cdot \text{K}$

**Planck's formula of black body radiation:**

$$I_\lambda(\lambda, T) := c_1 \cdot \frac{\lambda^{-5}}{e^{\frac{c_2}{\lambda \cdot T}} - 1}$$

$1000 \cdot (\text{\AA}) = 0.1 \cdot \mu\text{m}$        $I_\lambda(1000 \cdot \text{\AA}, 4000 \cdot \text{K}) = 8.94 \cdot \frac{\text{kW}}{\text{m}^3}$        $\lambda_0(T) := \frac{c_2}{5 \cdot T}$

$I_\lambda(1 \cdot \mu\text{m}, 6000 \cdot \text{K}) = 37411.94 \cdot \frac{\text{GW}}{\text{m}^3}$        $\sigma_{\text{SB}} = 56.7 \cdot \frac{\text{nW}}{\text{m}^2 \cdot \text{K}^4}$

if  $\lambda T \ll 1 \Rightarrow e^{\frac{c_2}{\lambda \cdot T}} \gg 1 \Rightarrow I_\lambda = c_1 \cdot \lambda^{-5} \cdot e^{-\frac{c_2}{\lambda \cdot T}}$

$$U(\omega, T) - U(\omega, 0) = \frac{\hbar \cdot \omega^3}{\pi^2 \cdot c^3 \cdot \left( \exp\left(\frac{\hbar \cdot \omega}{k \cdot T}\right) - 1 \right)}$$

Wien Displacement law

$$\lambda_{\text{max}}(T) := \frac{2.8978 \cdot 10^6}{T} \cdot \text{nm} \cdot \text{K}$$

$\lambda_{\text{max}}(6000 \cdot \text{K}) = 0.48 \cdot \mu\text{m}$

Color( $\lambda_{\text{max}}(6000 \cdot \text{K})$ ) = "Bleu"

Color( $\lambda_{\text{max}}(5000 \cdot \text{K})$ ) = "Yellow"

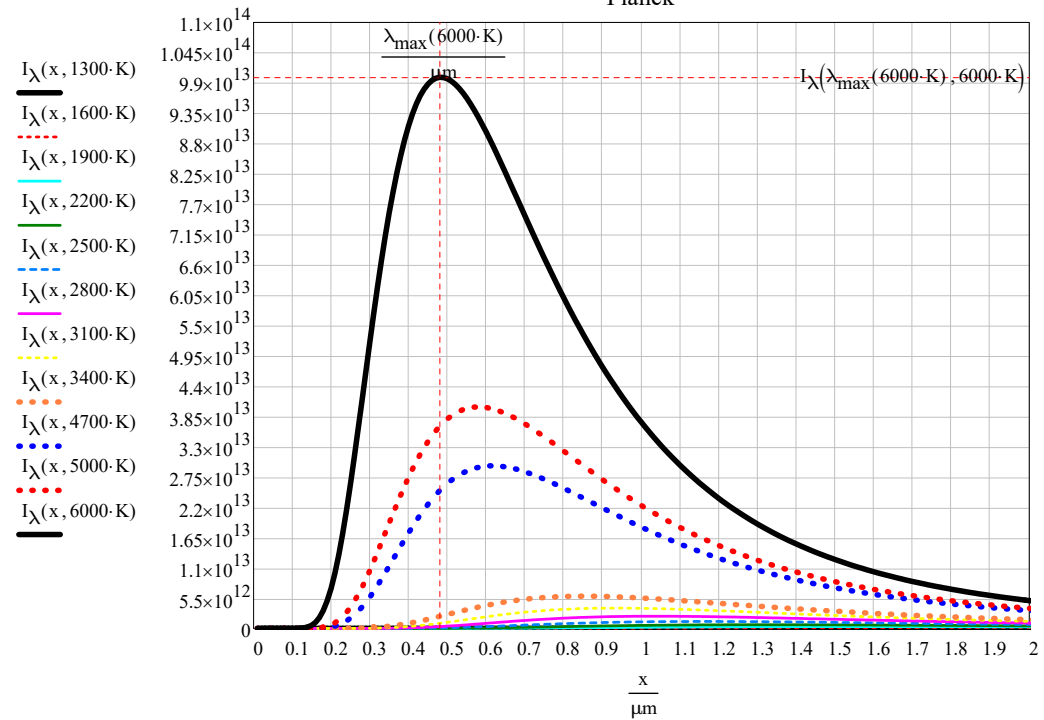
$\lambda_{\text{max}}(5000 \cdot \text{K}) = 0.58 \cdot \mu\text{m}$

Color( $\lambda_{\text{max}}(4700 \cdot \text{K})$ ) = "Red"

Essentially the solar spectrum is a black body radiation at 6050 K with power density:  $135.3 \cdot \frac{\text{mW}}{\text{cm}^3}$ .

$x := 0 \cdot \mu\text{m}, 0.01 \cdot \mu\text{m} \dots 4 \cdot \mu\text{m}$

## Planck



## Stefan-Boltzmann

$z = \lambda^{-1}$        $dz = -\lambda^{-2} \cdot d\lambda = -z^2 \cdot d\lambda$        $d\lambda = -\frac{dz}{z^2}$

$$\int_0^\infty c_1 \cdot \frac{\lambda^{-5}}{e^{\frac{c_2}{\lambda \cdot T}} - 1} d\lambda = - \int_\infty^0 c_1 \cdot \frac{z^5}{\left( e^{\frac{c_2 \cdot z}{T}} - 1 \right) \cdot z^2} dz = \int_0^\infty \frac{c_1 \cdot z^3}{e^{\frac{c_2 \cdot z}{T}} - 1} dz$$

$c_1 := c_1$        $T := T$        $\lambda := \lambda$        $c_2 := c_2$

$$c_1 \cdot \int_0^\infty \frac{z^3}{e^{\frac{c_2 \cdot z}{T}} - 1} dz \rightarrow \frac{\pi^4 \cdot T^4 \cdot c_1}{15 \cdot c_2^4}$$

$$\frac{\pi^4 \cdot T^4 \cdot c_1}{15 \cdot c_2^4} = \sigma \cdot T^4$$

$$\int_0^\infty c_1 \cdot \frac{\lambda^{-5}}{\frac{c_2}{e^{\lambda \cdot T} - 1}} d\lambda = \sigma_{SB} \cdot T^4$$

$$c_1 = 0 \frac{\text{kg} \cdot \text{m}^4}{\text{s}^3}$$

$$c_2 = 0.01 \cdot \text{m} \cdot \text{K}$$

$$\sigma_{SB} := \frac{\pi^2 \cdot k_B^4}{60 \cdot \hbar^3 \cdot c^2}$$

$$T := 300 \cdot \text{K} \quad a(T) := \frac{k_B \cdot T}{\hbar}$$

$$\frac{c_1}{c_2^4} = 8.73 \times 10^{-9} \frac{\text{kg}}{\text{s}^3 \cdot \text{K}^4}$$

$$\sigma_{SB} = 56.7 \cdot \frac{\text{nW}}{\text{m}^2 \cdot \text{K}^4}$$

$$a(T) = 3.93 \times 10^{13} \cdot \text{sec}^{-1}$$

$$\sigma_{SB} = 56.7 \cdot \frac{\text{nW}}{\text{m}^2 \cdot \text{K}^4}$$

$$E_{\text{tot}} = \int_0^\infty I_\lambda d\lambda = \sigma_{SB} \cdot T^4$$

The total emittance is given by the *Stefan-Boltzmann law*

$$E_{\text{tot}}(T) := \sigma_{SB} \cdot T^4$$

$$E_{\text{tot}}(T) = 459.24 \cdot \frac{\text{W}}{\text{m}^2}$$

## 22 Momentum Space Wave Function

$$dV = dx \cdot dy \cdot dz \quad d\mathbf{k} = dk_x \cdot dk_y \cdot dk_z \quad \mathbf{k} = k_x \cdot \mathbf{i}_x + k_y \cdot \mathbf{i}_y + k_z \cdot \mathbf{i}_z$$

Consider the Fourier transforms and the inverses of the wave function and of the potential:

$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{(2 \cdot \pi)^3}} \int f(\mathbf{k}) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} \quad f(\mathbf{k}) = \frac{1}{\sqrt{(2 \cdot \pi)^3}} \int \Psi(\mathbf{r}) \cdot e^{-i \cdot \mathbf{k} \cdot \mathbf{r}} dV \quad (22.1)$$

$$V(\mathbf{r}) = \int W(\mathbf{k}) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} \quad \lim_{r \rightarrow \infty} V(\mathbf{r}) = 0 \quad W(\mathbf{k}) = \frac{1}{(2 \cdot \pi)^3} \int V(\mathbf{r}) \cdot e^{-i \cdot \mathbf{k} \cdot \mathbf{r}} dV \quad (22.2)$$

$$\text{Substitute into the Schrödinger equation} \quad \frac{-\hbar^2}{2 \cdot m} \cdot \Delta \Psi(\mathbf{r}) + V(\mathbf{r}) \Psi(\mathbf{r}) = E \Psi(\mathbf{r}) \quad (22.3)$$

☑ Calculation of the MOMENTUM SPACE WAVE FUNCTION [3]

$$\left[ \frac{-\hbar^2}{2 \cdot m} \cdot \frac{1}{\sqrt{(2 \cdot \pi)^3}} \cdot \Delta \int f(\mathbf{k}) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} \dots \right] = E \cdot \frac{1}{\sqrt{(2 \cdot \pi)^3}} \int f(\mathbf{k}) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} \quad (22.4')$$

$$\left[ + \frac{1}{\sqrt{(2 \cdot \pi)^3}} \int W(\mathbf{k}) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} \int f(\mathbf{k}_1) \cdot e^{i \cdot \mathbf{k}_1 \cdot \mathbf{r}} d\mathbf{k}_1 \right]$$

$$\frac{-\hbar^2}{2 \cdot m} \int f(\mathbf{k}) \cdot \Delta e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} + \int W(\mathbf{k}) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} \int f(\mathbf{k}_1) \cdot e^{i \cdot \mathbf{k}_1 \cdot \mathbf{r}} d\mathbf{k}_1 = E \int f(\mathbf{k}) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} \quad (22.5')$$

consider the the second term on the left side:

$$\int W(\mathbf{k}) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} \int f(\mathbf{k}_1) \cdot e^{i \cdot \mathbf{k}_1 \cdot \mathbf{r}} d\mathbf{k}_1 = \int \int W(\mathbf{k}) \cdot f(\mathbf{k}_1) \cdot e^{i \cdot (\mathbf{k} + \mathbf{k}_1) \cdot \mathbf{r}} d\mathbf{k} d\mathbf{k}_1 \quad (22.6')$$

$$\text{replace } \mathbf{k}_2 = \mathbf{k} + \mathbf{k}_1 \quad \mathbf{k}_1 = \mathbf{k}_2 - \mathbf{k} \quad d\mathbf{k}_1 = d\mathbf{k}_2 \quad \mathbf{k} = \mathbf{k}_2 - \mathbf{k}_1 \quad d\mathbf{k} = d\mathbf{k}_2 \quad (22.7')$$

$$\text{obtaining} \int \int W(\mathbf{k}) \cdot f(\mathbf{k}_1) \cdot e^{i \cdot (\mathbf{k}_1 + \mathbf{k}) \cdot \mathbf{r}} d\mathbf{k} d\mathbf{k}_1 = \int \int W(\mathbf{k}_2 - \mathbf{k}_1) \cdot f(\mathbf{k}_1) \cdot e^{i \cdot \mathbf{k}_2 \cdot \mathbf{r}} d\mathbf{k}_1 d\mathbf{k}_2 \quad (22.8')$$

$$\mathbf{k}_2 = \mathbf{k} \quad (22.9')$$

$$\text{resulting} \int \int W(\mathbf{k}_2 - \mathbf{k}_1) \cdot f(\mathbf{k}_1) \cdot e^{i \cdot \mathbf{k}_2 \cdot \mathbf{r}} d\mathbf{k}_1 d\mathbf{k}_2 = \int \int W(\mathbf{k} - \mathbf{k}_1) \cdot f(\mathbf{k}_1) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k}_1 d\mathbf{k} \quad (22.10')$$

$$\text{furthermore } \Delta e^{i \cdot \mathbf{k} \cdot \mathbf{r}} = -\mathbf{k}^2 \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} \quad (22.11')$$

$$\frac{\hbar^2}{2 \cdot m} \int f(\mathbf{k}) \cdot \mathbf{k}^2 \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} + \int \int W(\mathbf{k} - \mathbf{k}_1) \cdot f(\mathbf{k}_1) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k}_1 d\mathbf{k} = E \int f(\mathbf{k}) \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} \quad (22.12')$$

$$\int \left[ \left( \frac{\hbar^2}{2 \cdot m} \cdot \mathbf{k}^2 - E \right) \cdot f(\mathbf{k}) + \int W(\mathbf{k} - \mathbf{k}_1) \cdot f(\mathbf{k}_1) d\mathbf{k}_1 \right] \cdot e^{i \cdot \mathbf{k} \cdot \mathbf{r}} d\mathbf{k} = 0 \quad (22.13')$$

$$\left( \frac{\hbar^2}{2 \cdot m} \cdot \mathbf{k}^2 - E \right) \cdot f(\mathbf{k}) + \int W(\mathbf{k} - \mathbf{k}_1) \cdot f(\mathbf{k}_1) d\mathbf{k}_1 = 0 \quad (22.14')$$

☑ Calculation of the MOMENTUM SPACE WAVE FUNCTION [3]

$$\text{integral equation} \int W(\mathbf{k} - \mathbf{k}_1) \cdot f(\mathbf{k}_1) d\mathbf{k}_1 = - \left( \frac{\hbar^2}{2 \cdot m} \cdot \mathbf{k}^2 - E \right) \cdot f(\mathbf{k}) \quad (22.4)$$

## 23 Representations theory

Euclidean representation:  $\langle x | \Psi \rangle = \Psi(x)$ ,  $\langle \Psi | x \rangle = \Psi(x)^*$ ,

k representation:  $\langle k | \Psi \rangle = \Psi(k)$ ,  $\langle \Psi | k \rangle = \Psi(k)^*$ ,

p representation:  $\langle p | \Psi \rangle = \Psi(p)$ ,  $\langle \Psi | p \rangle = \Psi(p)^*$ ,

$$\text{Closure relation: } \mathbf{P}_A = \sum_{j=1}^N |j\rangle\langle j| + \int_{\xi_1}^{\xi_2} |\xi\rangle d\xi \langle \xi| = 1 \quad (10.12)$$

$$\mathbf{P}_A \mathbf{H} = \sum_{j=1}^N |j\rangle\langle j| \mathbf{H} + \int_{\xi_1}^{\xi_2} |\xi\rangle d\xi \langle \xi| \mathbf{H} = \sum_{j=1}^N \frac{|j\rangle\langle j|}{\lambda_j} + \frac{\int_{\xi_1}^{\xi_2} |\xi\rangle d\xi \langle \xi|}{\lambda}$$

$$\mathbf{P}_A = \sum_{j=1}^N |j\rangle\langle j| = 1$$

$$\mathbf{H} | \psi \rangle = E_k | \psi \rangle$$

$$(z - \mathbf{H}) | \psi \rangle = (z - E_k) | \psi \rangle$$

$$(z - \mathbf{H}) \cdot \mathbf{P}_A | \psi \rangle = (z - E_k) \cdot \mathbf{P}_A | \psi \rangle$$

apply the closure relation (10.12) assuming that there is no continuous spectrum

$$(z - \mathbf{H}) \cdot \sum_{j=1}^N |j\rangle\langle j| \psi \rangle = (z - E_k) \cdot \sum_{j=1}^N |j\rangle\langle j| \psi \rangle$$

$$(z - \mathbf{H})^{-1} \cdot \sum_{j=1}^N |j\rangle\langle j| \psi \rangle = \frac{1}{(z - E_k)} \cdot \sum_{j=1}^N |j\rangle\langle j| \psi \rangle$$

$$(z - \mathbf{H})^{-1} \cdot \sum_{j=1}^N |j\rangle\langle j| = \frac{1}{(z - E_k)} \cdot \sum_{j=1}^N |j\rangle\langle j| = \sum_{j=1}^N \frac{|j\rangle\langle j|}{z - E_k} = G(z)$$

$$\text{Green function: } G(z) = \sum_{j=1}^N \frac{|j\rangle\langle j|}{z - E_k}$$

## 24 Time evolution of the average value of an observable [4]

$$\frac{d}{dt} \langle \mathbf{A} \rangle = \frac{1}{i\hbar} \cdot (\langle [ \mathbf{A}, \mathbf{H} ] \rangle) + \left\langle \frac{\partial \mathbf{A}}{\partial t} \right\rangle \quad (24.1)$$

□ Demonstration of 23.1)

Consider the definition of average value:

$$\langle \mathbf{A} \rangle = \langle \psi | \mathbf{A} | \psi \rangle = \int \Psi(\tau)^* \cdot \mathbf{A} \cdot \Psi(\tau) d\tau \quad (24.2)$$

and calculate the expectation value derivative:

$$\frac{d}{dt} \langle \mathbf{A} \rangle = \frac{d}{dt} \langle \psi | \mathbf{A} | \psi \rangle \quad (24.3)$$

$$\text{calculation result: } \frac{d}{dt} \langle \mathbf{A} \rangle = \left( \frac{\partial}{\partial t} \langle \psi | \right) \mathbf{A} | \psi \rangle + \langle \psi | \frac{\partial \mathbf{A}}{\partial t} | \psi \rangle + \langle \psi | \mathbf{A} \frac{\partial}{\partial t} | \psi \rangle \quad (24.4)$$

$$\text{knowing that: } i\hbar \cdot \frac{\partial}{\partial t} | \psi \rangle = \mathbf{H} | \psi \rangle \quad \text{and} \quad -i\hbar \cdot \frac{\partial}{\partial t} \langle \psi | = \langle \psi | \mathbf{H}^\dagger \quad (24.5)$$

$$\text{from which } \frac{\partial}{\partial t} | \psi \rangle = \frac{1}{i\hbar} \cdot \mathbf{H} | \psi \rangle \quad \text{and} \quad \frac{\partial}{\partial t} \langle \psi | = \langle \psi | \mathbf{H}^\dagger \cdot \frac{1}{-i\hbar} \quad (24.6)$$

$$\langle \psi | \frac{\partial \mathbf{A}}{\partial t} | \psi \rangle = \left\langle \frac{\partial \mathbf{A}}{\partial t} \right\rangle$$

after a substitution in 22.4), I get

$$\begin{aligned} \frac{d}{dt} \langle \mathbf{A} \rangle &= \left( \frac{\partial}{\partial t} \langle \psi | \right) \mathbf{A} (| \psi \rangle) + \langle \psi | \mathbf{A} \frac{\partial}{\partial t} | \psi \rangle \dots = \left( \langle \psi | \mathbf{H}^\dagger \cdot \frac{1}{-i\hbar} \right) \mathbf{A} (| \psi \rangle) \dots \\ &+ \left\langle \frac{\partial \mathbf{A}}{\partial t} \right\rangle + \langle \psi | \mathbf{A} \left( \frac{1}{i\hbar} \cdot \mathbf{H} | \psi \right) \rangle + \left\langle \frac{\partial \mathbf{A}}{\partial t} \right\rangle \end{aligned}$$

$$\text{so that } \frac{d}{dt} \langle \mathbf{A} \rangle = \left( \langle \psi | \mathbf{H}^\dagger \cdot \frac{1}{-i\hbar} \right) \mathbf{A} (| \psi \rangle) + \langle \psi | \mathbf{A} \left( \frac{1}{i\hbar} \cdot \mathbf{H} | \psi \right) \rangle + \left\langle \frac{\partial \mathbf{A}}{\partial t} \right\rangle$$

$$\frac{d}{dt} \langle \mathbf{A} \rangle = -\frac{1}{i\hbar} \left( \langle \psi | \mathbf{H}^\dagger \cdot \mathbf{A} | \psi \rangle \right) + \frac{1}{i\hbar} \left( \langle \psi | \mathbf{H} \cdot \mathbf{A} | \psi \rangle \right) + \left\langle \frac{\partial \mathbf{A}}{\partial t} \right\rangle$$

$$\text{namely } \frac{d}{dt} \langle \mathbf{A} \rangle = \frac{1}{i\hbar} \cdot \left( \langle \psi | \mathbf{A} \cdot \mathbf{H} | \psi \rangle - \langle \psi | \mathbf{H}^\dagger \cdot \mathbf{A} | \psi \rangle \right) + \left\langle \frac{\partial \mathbf{A}}{\partial t} \right\rangle \quad (24.7)$$

Self adjoint Operator (Hermitian):  $\mathbf{H} = \mathbf{H}^\dagger$

$$\frac{d}{dt} \langle \mathbf{A} \rangle = \frac{1}{i\hbar} \cdot \langle \psi | (\mathbf{A} \cdot \mathbf{H} - \mathbf{H} \cdot \mathbf{A}) | \psi \rangle + \left\langle \frac{\partial \mathbf{A}}{\partial t} \right\rangle \quad (24.8)$$

$$\frac{d}{dt} \langle \mathbf{A} \rangle = \frac{1}{i\hbar} \cdot (\langle [ \mathbf{A}, \mathbf{H} ] \rangle) + \left\langle \frac{\partial \mathbf{A}}{\partial t} \right\rangle$$

$$\frac{d^2}{dt^2} \langle \mathbf{A} \rangle = -\frac{1}{\hbar^2} \langle [[\mathbf{A}, \mathbf{H}], \mathbf{H}] \rangle + \frac{1}{i\hbar} \left\langle \frac{d}{dt} [\mathbf{A}, \mathbf{H}] \right\rangle + \frac{\partial}{\partial t} \left\langle \frac{\partial}{\partial t} \mathbf{A} \right\rangle \quad (24.9)$$

$$\frac{d}{dt} \langle [\mathbf{A}, \mathbf{H}] \rangle = \frac{1}{i\hbar} \cdot (\langle [[\mathbf{A}, \mathbf{H}], \mathbf{H}] \rangle) + \left\langle \frac{\partial}{\partial t} [\mathbf{A}, \mathbf{H}] \right\rangle$$

$$\frac{d^2}{dt^2} \langle \mathbf{A} \rangle = \frac{1}{i\hbar} \cdot \frac{d}{dt} \langle [\mathbf{A}, \mathbf{H}] \rangle + \frac{\partial}{\partial t} \left\langle \frac{\partial}{\partial t} \mathbf{A} \right\rangle$$

$$\frac{1}{i\hbar} \cdot \frac{d}{dt} \langle [\mathbf{A}, \mathbf{H}] \rangle + \frac{\partial}{\partial t} \left\langle \frac{\partial}{\partial t} \mathbf{A} \right\rangle = \frac{1}{i\hbar} \cdot \left[ \frac{1}{i\hbar} \cdot (\langle [[\mathbf{A}, \mathbf{H}], \mathbf{H}] \rangle) + \left\langle \frac{\partial}{\partial t} [\mathbf{A}, \mathbf{H}] \right\rangle \right] + \frac{\partial}{\partial t} \left\langle \frac{\partial}{\partial t} \mathbf{A} \right\rangle$$

$$\frac{d^2}{dt^2} \langle \mathbf{A} \rangle = -\frac{1}{\hbar^2} \cdot (\langle [[\mathbf{A}, \mathbf{H}], \mathbf{H}] \rangle) + \frac{1}{i\hbar} \cdot \left( \left\langle \frac{d}{dt} [\mathbf{A}, \mathbf{H}] \right\rangle \right) + \frac{\partial}{\partial t} \left\langle \frac{\partial}{\partial t} \mathbf{A} \right\rangle$$

$$\frac{d^2}{dt^2} \langle \mathbf{A} \rangle = -\frac{1}{\hbar^2} \cdot (\langle [[\mathbf{A}, \mathbf{H}], \mathbf{H}] \rangle) + \frac{1}{i\hbar} \cdot \left( \left\langle \frac{d}{dt} [\mathbf{A}, \mathbf{H}] \right\rangle \right) - \frac{1}{i\hbar} \cdot \frac{\partial}{\partial t} \langle [\mathbf{A}, \mathbf{H}] \rangle + \frac{d^2}{dt^2} \langle \mathbf{A} \rangle$$

Eq. 24.1 can be rewritten as:  $\left\langle \frac{\partial}{\partial t} \mathbf{A} \right\rangle = -\frac{1}{i\hbar} \langle [\mathbf{A}, \mathbf{H}] \rangle + \frac{d}{dt} \langle \mathbf{A} \rangle \quad (24.10)$

For a system in stationary state, of energy  $E(\omega) := \hbar \cdot \omega$

$$|\Psi\rangle = e^{-i \cdot \frac{E \cdot t}{\hbar}} |\psi\rangle$$

$$E \cdot \psi \cdot e^{-i \cdot \frac{E \cdot t}{\hbar}} = \mathbf{H} \left( \psi \cdot e^{-i \cdot \frac{E \cdot t}{\hbar}} \right)$$

**Schrödinger equation for the stationary state**  $\mathbf{H} \cdot \psi = E \cdot \psi \quad \mathbf{H} |\psi_k\rangle = E_k |\psi_k\rangle$

The observable is a motion's constant when the operator isn't time dependent. This happens if and only if its average isn't time dependent.

**Theorem:** *a necessary and sufficient condition that a time independent observable be a motion's constant, is that the Hamiltonian commute with it. It follows that all statistical moments are time independent as well.*

*The set of all time independent variables commuting with the Hamiltonian (compatibility) coincide with the motion's constants.*

## 25 Conservation Laws [4]

For a particle in a scalar potential:

Probability density  $P = \psi^* \cdot \psi \quad (25.1)$

Probability current density  $\mathbf{J} = \frac{\hbar}{2 \cdot m \cdot i} \cdot [\psi^* \cdot \nabla \psi - (\nabla \psi)^* \cdot \psi] \quad (25.2)$

Continuity law  $\nabla \cdot \mathbf{J} + \frac{\partial}{\partial t} P = 0 \quad (25.3)$

Energy Flux vector  $\mathbf{S} = -\frac{\hbar^2}{2 \cdot m} \cdot \left[ \frac{\partial}{\partial t} \psi^* \cdot \nabla \psi - \frac{\partial}{\partial t} \psi \cdot \nabla (\psi^*) \right] \quad (25.4)$

Energy density  $W = \frac{\hbar^2}{2 \cdot m} \cdot [\nabla (\psi^*) \cdot \nabla \psi + \psi^* \cdot \nabla \psi] \quad (25.5)$

## 26 Commutation relations of Angular Momentum [4]

(Classical mechanics  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ )

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \leftrightarrow -i\hbar \cdot \mathbf{r} \times \nabla, \quad (26.1)$$

$$[\mathbf{q}_i, \mathbf{A}(\mathbf{p}_i, \mathbf{q}_i)] = -i\hbar \cdot \frac{\partial}{\partial \mathbf{q}_i} \mathbf{A}(\mathbf{p}_i, \mathbf{q}_i) \quad (26.2)$$

$$[\mathbf{L}_x, \mathbf{L}_y] = i\hbar \cdot \mathbf{L}_z \quad (26.3)$$

$$[\mathbf{L}_y, \mathbf{L}_z] = i\hbar \cdot \mathbf{L}_x \quad (26.4)$$

$$[\mathbf{L}_z, \mathbf{L}_x] = i\hbar \cdot \mathbf{L}_y \quad (26.5)$$

$$[\mathbf{L}_z, \mathbf{L}_x^2] = i\hbar \cdot (\mathbf{L}_y \cdot \mathbf{L}_x + \mathbf{L}_x \cdot \mathbf{L}_y) \quad (26.6)$$

$$[\mathbf{L}_z, \mathbf{L}_y^2] = i\hbar \cdot (\mathbf{L}_y \cdot \mathbf{L}_x + \mathbf{L}_x \cdot \mathbf{L}_y) \quad (26.7)$$

$$[\mathbf{L}_z, \mathbf{L}_z^2] = 0 \quad (26.8)$$

$\mathbf{u}$  is a unit vector  $[\mathbf{u} \cdot \mathbf{L}, \mathbf{p}] = -i\hbar \cdot (\mathbf{i}_x \times \mathbf{p}) \quad (26.9)$

$\mathbf{u}$  is a unit vector  $[\mathbf{u} \cdot \mathbf{L}, \mathbf{r}] = -i\hbar \cdot (\mathbf{i}_x \times \mathbf{r}) \quad (26.10)$

$\mathbf{u}$  is a unit vector  $[\mathbf{u} \cdot \mathbf{L}, \mathbf{p}^2] = 0 \quad (26.11)$

$\mathbf{u}$  is a unit vector  $[\mathbf{u} \cdot \mathbf{L}, \mathbf{r}^2] = 0 \quad (26.12)$

$\mathbf{u}$  is a unit vector  $[\mathbf{u} \cdot \mathbf{L}, \mathbf{r} \cdot \mathbf{p}] = 0 \quad (26.13)$

Spherical coordinates  $(r, \theta, \varphi)$   $\mathbf{p}_r = \frac{\hbar}{i} \cdot \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \quad (26.14)$

Classical mechanics  $\mathbf{p}^2 = \mathbf{p}_r^2 + \frac{\mathbf{L}^2}{r^2} \quad (26.15)$

$$\mathbf{L}^2 = \frac{\hbar^2}{\sin(\theta)^2} \cdot \left[ \sin(\theta) \cdot \left[ \frac{\partial}{\partial \theta} \left( \sin(\theta) \cdot \frac{\partial}{\partial \theta} \right) \right] + \frac{\partial^2}{\partial \varphi^2} \right] \quad (26.16)$$

$$\mathbf{L}^2 Y(l, m, \theta, \varphi) = l(l+1) \cdot \hbar^2 \cdot Y(l, m, \theta, \varphi) \quad l = 0, 1, 2, \dots, \infty \quad (26.17)$$

$$\mathbf{L}_z Y(l, m, \theta, \varphi) = m \cdot \hbar \cdot Y(l, m, \theta, \varphi) \quad m = -l, -l+1, \dots, l \quad (26.18)$$

$$P_l(\cos(\gamma_0)) = \frac{4 \cdot \pi}{2 \cdot l + 1} \cdot \sum_{j=-l}^l (Y(l, j, \Theta, \Phi) * Y(l, j, \theta, \varphi)) \quad (26.19)$$

☐ Angular moment theorem

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \leftrightarrow \frac{\hbar}{i} \cdot (\mathbf{r} \times \nabla) \quad \langle \mathbf{L} \rangle = \frac{\hbar}{i} \cdot \int \langle \psi | \mathbf{r} \times \nabla | \psi \rangle dV$$

**Angular moment theorem** momentum  $\mathbf{T}$  of the force  $\mathbf{F} = -\nabla U$ :

$$\mathbf{T} = \mathbf{r} \times \mathbf{F} = -(\mathbf{r} \times \nabla U(\mathbf{r})) = \frac{\partial}{\partial t} \mathbf{L} \quad \langle \mathbf{T} \rangle = - \int \langle \psi | (\mathbf{r} \times \nabla U(\mathbf{r})) | \psi \rangle dV$$

$$\frac{\partial}{\partial t} \langle \mathbf{L} \rangle = \frac{\hbar}{i} \cdot \int \frac{\partial}{\partial t} \langle \psi | \mathbf{r} \times \nabla | \psi \rangle + \langle \psi | \mathbf{r} \times \nabla \frac{\partial}{\partial t} | \psi \rangle dV$$

$$\frac{\partial}{\partial t} \langle \mathbf{L} \rangle = \frac{\hbar}{i} \cdot \int \frac{\partial}{\partial t} \langle \psi | \mathbf{r} \times \nabla | \psi \rangle + \mathbf{r} \times \langle \psi | \nabla \frac{\partial}{\partial t} | \psi \rangle dV$$

$$\nabla \langle \psi | \frac{\partial}{\partial t} | \psi \rangle = \langle \psi | \nabla \frac{\partial}{\partial t} | \psi \rangle + \left( \frac{\partial}{\partial t} | \psi \rangle \right) \nabla \langle \psi |$$

$$\langle \psi | \nabla \left( \frac{\partial}{\partial t} | \psi \rangle \right) = \nabla \left( \langle \psi | \frac{\partial}{\partial t} | \psi \rangle \right) - \left( \frac{\partial}{\partial t} | \psi \rangle \right) \nabla \langle \psi |$$

$$\frac{\partial}{\partial t} \langle \mathbf{L} \rangle = \frac{\hbar}{i} \cdot \int \frac{\partial}{\partial t} \langle \psi | \mathbf{r} \times \nabla | \psi \rangle + \mathbf{r} \times \left[ \nabla \left( \langle \psi | \frac{\partial}{\partial t} | \psi \rangle \right) - \left( \frac{\partial}{\partial t} | \psi \rangle \right) \nabla \langle \psi | \right] dV$$

$$\int \mathbf{r} \times \nabla f(\mathbf{r}) dV = 0$$

☐ Angular moment theorem



A vector operator  $\mathbf{J}$  is an angular momentum if its components are observables satisfying the following commutation relations:

$$\mathbf{J} = J_x \cdot \mathbf{i}_x + J_y \cdot \mathbf{i}_y + J_z \cdot \mathbf{i}_z \quad (26.20)$$

$$[J_x, J_y] = i \cdot \hbar \cdot J_z \quad (26.21)$$

$$[J_y, J_z] = i \cdot \hbar \cdot J_x \quad (26.22)$$

$$[J_z, J_x] = i \cdot \hbar \cdot J_y \quad (26.23)$$

If  $\mathbf{a}$  and  $\mathbf{b}$  are any two vectors (or any two vector operators that commute with each other and also with  $\mathbf{J}$ ) I get

$$[\mathbf{a} \cdot \mathbf{J}, \mathbf{b} \cdot \mathbf{J}] = i \cdot \hbar \cdot (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{J} \quad (26.24)$$

$$[\mathbf{J}, \mathbf{J}^2] = 0 \quad (26.25)$$

$$[f(\mathbf{J}_\alpha), \mathbf{J}^2] = 0 \quad (26.26)$$

Hermitian conjugated operators:  $\mathbf{J}_+ = J_x + i \cdot J_y$      $\mathbf{J}_- = J_x - i \cdot J_y$

$$[J_z, J_+] = \hbar \cdot J_+ \quad (26.27)$$

$$[J_z, J_-] = -\hbar \cdot J_- \quad (26.28)$$

$$[J_+, J_-] = 2 \cdot \hbar \cdot J_z \quad (26.29)$$

Demonstration of (25.27), (25.28), (25.29)

$$[J^2, J_+] = [J^2, J_-] = [J^2, J_z] = 0 \quad (26.30)$$

$$J^2 = \frac{1}{2} \cdot (J_+ \cdot J_- + J_- \cdot J_+) + J_z^2 \quad (26.31)$$

$$J_- \cdot J_+ = J^2 - J_z \cdot (J_z + 1) \quad (26.32)$$

$$J_+ \cdot J_- = J^2 - J_z \cdot (J_z - 1) \quad (26.33)$$

## 27 Charged Elemental Particle (Q) in an Electromagnetic Field

MKS-GAUSS

Electric field

Since  $\nabla \cdot \mathbf{B}(x, y, z, t) = 0$ , (Electromagnetics eq. 4), a necessary and sufficient condition for *solenoidal fields* is  $\nabla \cdot \mathbf{V} = 0 \Rightarrow \mathbf{V} = \nabla \times \mathbf{U} \Rightarrow \nabla \cdot (\nabla \times \mathbf{U}) = 0$

**Option 1)** so that I can place  $\mathbf{B}(x, y, z, t) = \nabla \times \mathbf{A}(x, y, z, t)$      $[A] = \frac{\text{Wb}}{\text{m}}$

**Option 2)** if I choose instead  $\mathbf{H}(x, y, z, t) = \nabla \times \mathbf{A}(x, y, z, t)$  then the unit is  $[A] = \text{Ampère}$

**As a result of the Option 2)**  $\mathbf{B}(x, y, z, t) = \mu \cdot \nabla \times \mathbf{A}(x, y, z, t)$

Next I would always consider **Option 1)**. Now substitute a1) into the first Maxwell equation, here rewritten:

$$\nabla \times \mathbf{E}(x, y, z, t) = -\frac{\partial}{\partial t} \mathbf{B}(x, y, z, t)$$

obtaining:  $\nabla \times \mathbf{E}(x, y, z, t) = -\frac{\partial}{\partial t} (\nabla \times \mathbf{A}(x, y, z, t))$

leaving the right hand side free, I have

$$\nabla \times \mathbf{E}(x, y, z, t) + \frac{\partial}{\partial t} (\nabla \times \mathbf{A}(x, y, z, t)) = 0 \cdot \frac{\text{T}}{\text{s}} = 0 \cdot \frac{\text{volt}}{\text{m}^2}$$

and collecting the rotor operators, results

$$\nabla \times \left( \mathbf{E}(x, y, z, t) + \frac{\partial}{\partial t} \mathbf{A}(x, y, z, t) \right) = 0 \cdot \frac{\text{volt}}{\text{m}^2} \quad [A] = \frac{\text{Wb}}{\text{m}}$$

Generally if  $\nabla \times \mathbf{U} = 0 \Rightarrow \mathbf{U} = -\nabla \varphi$      $\nabla \times \nabla \varphi = 0$

$\nabla \times \mathbf{V} = 0 \Rightarrow \mathbf{V} = \nabla \varphi$     Lamellar field (conservative and irrotational)

$\mathbf{V} \cdot (\nabla \times \mathbf{V}) = 0$     Composed lamellar field

resulting:  $\mathbf{E}(x, y, z, t) + \frac{\partial}{\partial t} \mathbf{A}(x, y, z, t) = -\nabla \varphi(x, y, z, t)$

Electric field

The electric field is linked to the vector potential by the relation:

$$\frac{\text{volt}}{\text{m}} \quad \mathbf{E}(\mathbf{R}, t) = -\nabla \varphi(\mathbf{R}, t) - \frac{\partial}{\partial t} \mathbf{A}(\mathbf{R}, t) \quad \frac{\text{Wb}}{\text{m} \cdot \text{sec}} = 1 \cdot \frac{\text{volt}}{\text{m}} \quad (27.1)$$

$$\frac{\partial}{\partial t} \mathbf{A}(\mathbf{R}, t) = \nabla \mathbf{A}(\mathbf{R}, t) \cdot \frac{\partial}{\partial t} \mathbf{R} = \mathbf{v} \cdot \nabla \mathbf{A}(\mathbf{R}, t) \quad (27.2)$$

$$\frac{\text{volt}}{\text{m}} \quad \mathbf{E}(\mathbf{R}, t) = -\nabla \varphi(\mathbf{R}, t) - \mathbf{v} \cdot \nabla \mathbf{A}(\mathbf{R}, t) \quad \frac{\text{Wb}}{\text{m} \cdot \text{sec}} = 1 \cdot \frac{\text{volt}}{\text{m}} \quad (27.1')$$

$$\mathbf{E}(\mathbf{R}, t) = -\nabla(\varphi(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t))$$

verify

Consider the electric charge  $Q$  immersed in an electromagnetic field. It is subject to the Lorentz force:

$$\mathbf{F} = Q \cdot (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \quad (27.3)$$

Substitute in it eq. 27.1) and the option 27.a1) (Option 1). Results:

$$\mathbf{F} = m \cdot \mathbf{q}'' = \mathbf{p}' = Q \cdot \left[ -\nabla \varphi - \frac{\partial}{\partial t} \mathbf{A} + \mathbf{v} \times (\nabla \times \mathbf{A}) \right] \quad (27.4)$$

$$\mathbf{v} \times (\nabla \times \mathbf{A}) = \nabla(\mathbf{v} \cdot \mathbf{A}) - [(\mathbf{v} \cdot \nabla) \cdot \mathbf{A} + (\mathbf{A} \cdot \nabla) \cdot \mathbf{v} + \mathbf{A} \times (\nabla \times \mathbf{v})] \quad (27.5)$$

$$\frac{\partial}{\partial t} \mathbf{A} = \mathbf{v} \cdot \nabla \mathbf{A} \quad (27.2)$$

$$\mathbf{F} = Q \cdot [-\nabla \varphi - \mathbf{v} \cdot \nabla \mathbf{A} + \nabla(\mathbf{v} \cdot \mathbf{A}) - [(\mathbf{v} \cdot \nabla) \cdot \mathbf{A} + (\mathbf{A} \cdot \nabla) \cdot \mathbf{v} + \mathbf{A} \times (\nabla \times \mathbf{v})]] \quad (27.6)$$

furthermore, collecting the gradient operators, I can write:

$$\mathbf{E}(\mathbf{R}, t) = -\nabla(\varphi(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)) = -\nabla(\Theta_p) \quad (27.7)$$

so that I can define the scalar potential:  $\Theta_p(\mathbf{R}, t) = V(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)$  (27.8)

$$\text{while the potential energy is } U(\mathbf{R}, t) = Q \cdot (V(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)) \quad Q = \pm q_e \quad (27.9)$$

which is useful to define the Lagrangian.

$$\text{Lagrangian coordinates: } \mathbf{p} = m \cdot \mathbf{q}' \quad \mathbf{p}' = m \cdot \mathbf{q}'' \quad \mathbf{q} = \mathbf{r} \quad (27.10)$$

$$\mathbf{F} = m \cdot \mathbf{q}'' = \mathbf{p}' \quad \mathbf{q}' = \frac{\mathbf{p}}{m} \quad (27.11)$$

Cinematic moment (A is the potential vector)

$$T = \frac{\mathbf{p}^2}{2 \cdot m} = \frac{\mathbf{p} \cdot m \cdot \mathbf{q}'}{2 \cdot m} = \frac{\mathbf{p} \cdot \mathbf{q}'}{2} \quad (27.12)$$

$$U = Q \cdot (V(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)) + \Theta(\mathbf{r}) \quad (27.13)$$

$$\text{Classical Lagrangian } \mathbf{L} = T - U = \frac{\mathbf{p} \cdot \mathbf{q}'}{2} - Q \cdot (V(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)) - \Theta(\mathbf{r}) \quad U = T - \mathbf{L} \quad (27.14)$$

$$\mathbf{L} = \frac{\mathbf{p} \cdot \mathbf{q}'}{2} - Q \cdot (V(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)) - \Theta(\mathbf{r}) = \frac{\mathbf{p}^2}{2 \cdot m} - Q \cdot (V + \mathbf{v} \cdot \mathbf{A}) - \Theta(\mathbf{r}) \quad (27.15)$$

Classical Hamiltonian in an electromagnetic field:

$$U = T - \mathbf{L} \quad \mathbf{H} = T + U = 2 \cdot T - \mathbf{L} = \mathbf{p} \cdot \mathbf{q}' - \frac{\mathbf{p} \cdot \mathbf{q}'}{2} + Q \cdot (V(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)) + \Theta(\mathbf{r}) \quad (27.16)$$

$$\mathbf{H} = \frac{\mathbf{p} \cdot \mathbf{q}'}{2} + Q \cdot (V(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)) + \Theta(\mathbf{r}) \quad (27.17)$$

Classical Lagrangian for one electron ( $\Phi=0, Q=-q_e$ ) in an electromagnetic field:

$$\mathbf{L} = \frac{\mathbf{p} \cdot \mathbf{q}'}{2} + q_e \cdot (V(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)) \quad (27.18)$$

Classical Hamiltonian for one electron ( $\Phi=0, Q=-q_e$ ) in an electromagnetic field:

$$\mathbf{H} = \frac{\mathbf{p} \cdot \mathbf{q}'}{2} - q_e \cdot (V(\mathbf{R}, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{R}, t)) + \Theta(\mathbf{r}) \quad (27.19)$$

$$\text{Scalar potential due to electrostatic field } V(\mathbf{r}) = - \int \mathbf{E}(\mathbf{r}) \, d\mathbf{r}, \text{ or } \mathbf{E}(\mathbf{r}) = -\nabla V(\mathbf{r}) \quad (27.20)$$

The Potential due to non electromagnetic forces is indicated with  $\Theta(\mathbf{r})$

Electromagnetic vector potential  $\mathbf{A}$ , magnetic induction  $\mathbf{B} = \nabla \times \mathbf{A}$  (T). In a system of currents,  $\mathbf{A}$  is the solution of the Helmholtz equation

$$\nabla^2 \mathbf{A}(x, y, z) + k^2 \cdot \mathbf{A}(x, y, z) = -\mathbf{J}_{\sigma}(x, y, z), \quad k^2 = \omega^2 \cdot \mu \cdot \epsilon \quad (27.21)$$

$$\mathbf{A}(x, y, z) = \frac{1}{4 \cdot \pi} \iiint \mathbf{J}(\mathbf{p}_1) \cdot \frac{e^{-i \cdot (|\mathbf{p} - \mathbf{p}_1|)}}{|\mathbf{p} - \mathbf{p}_1|} \, dx \, dy \, dz \quad (27.22)$$

Apply the quantization rules to the classical Hamiltonian of one electron ( $\Phi=0, Q=-q_e$ ) in an electromagnetic field:

Quantization rules (substitute to each classical operator of the Hamiltonian the corresponding Quantum Operator) when the quantum system possesses a classical analogue:

Classical Operator	Quantized Operator acting on kets or eigenfunctions
--------------------	---

$$\mathbf{p} \leftrightarrow -i \cdot \hbar \cdot \nabla,$$

$$\mathbf{q}' \leftrightarrow -i \cdot \frac{\hbar}{m} \cdot \nabla$$

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \leftrightarrow -i \cdot \hbar \cdot \mathbf{r} \times \nabla,$$

$$\mathbf{L}_x \leftrightarrow -i \cdot \hbar \cdot \left( y \cdot \frac{\partial}{\partial z} - z \cdot \frac{\partial}{\partial y} \right),$$

$$\mathbf{L}_y \leftrightarrow -i \cdot \hbar \cdot \left( z \cdot \frac{\partial}{\partial x} - x \cdot \frac{\partial}{\partial z} \right),$$

$$\mathbf{L}_z \leftrightarrow -i \cdot \hbar \cdot \left( x \cdot \frac{\partial}{\partial y} - y \cdot \frac{\partial}{\partial x} \right),$$

$$\mathbf{p}^2 \leftrightarrow -\hbar^2 \cdot \Delta,$$

$$\frac{\mathbf{p} \cdot \mathbf{q}'}{2} = \frac{\mathbf{p}^2}{2 \cdot m} \leftrightarrow \frac{-\hbar^2}{2 \cdot m} \cdot \Delta$$

$$\text{Energy } E \leftrightarrow i \cdot \hbar \cdot \frac{\partial}{\partial t}$$

$$\mathbf{r}^2 = (\mathbf{r} \times \mathbf{p}) \cdot (\mathbf{r} \times \mathbf{p}) = r^2 \cdot (\mathbf{p}^2 - p_r^2) \leftrightarrow r^2 \cdot \left[ -\hbar^2 \cdot \Delta + \hbar^2 \cdot \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \right] \text{ Sph. coord.}$$

$$\mathbf{r} \cdot \mathbf{p} \leftrightarrow -i \cdot \hbar \cdot r \cdot \frac{\partial}{\partial r} = -i \cdot \hbar \cdot r \cdot \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \text{ Sph. coord.}$$

$$\mathbf{s} \cdot \mathbf{p} \leftrightarrow \nabla \times \quad [4] \text{ pag.: 551}$$

### Classical Hamiltonian for a non relativistic particle of rest mass m:

how do I get the quantized Hamiltonian? I substitute to each classical operator the one given by the table of the correspondences (at first only the energy E).

Classical mechanical energy  $E = T + U = \mathbf{H}$ . In QM, to E and  $\mathbf{H}$  correspond to each one an operators acting on a ket:

$$\mathbf{E} | \Psi \rangle = \mathbf{H} | \Psi \rangle. \quad (27.24)$$

Namely, applying t

$$\mathbf{H} = \frac{\mathbf{p}^2}{2 \cdot m} - q_e \cdot \left( V + \frac{m \cdot \mathbf{v} \cdot \mathbf{A}(\mathbf{q}, t)}{m} \right) + \Theta(\mathbf{r}) = \frac{\mathbf{p}^2}{2 \cdot m} - q_e \cdot V - \frac{q_e \cdot \mathbf{p} \cdot \mathbf{A}(\mathbf{q}, t)}{m} + \Theta(\mathbf{r}) \quad (27.25)$$

$$\begin{array}{ccc} \text{Classical Hamiltonian} & \leftrightarrow & \text{QM Hamiltonian} \\ \downarrow & & \downarrow \end{array} \quad (27.26)$$

$$\mathbf{H} = \frac{\mathbf{p}^2}{2 \cdot m} - q_e \cdot V - \frac{q_e \cdot \mathbf{p} \cdot \mathbf{A}(\mathbf{q}, t)}{m} + \Theta(\mathbf{r}) \quad \leftrightarrow \quad \mathbf{H} = \frac{\hbar^2}{2 \cdot m} \cdot \nabla^2 + \frac{i \cdot q_e \cdot \hbar}{m} \cdot \mathbf{A} \cdot \nabla - q_e \cdot V + \Theta(\mathbf{r}) \quad (27.27)$$

$$\text{in fact for the scalar product between } \mathbf{p} \text{ and } \mathbf{A}, \text{ I can write: } \quad \mathbf{p} \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{p} \leftrightarrow -i \cdot \hbar \cdot \mathbf{A} \cdot \nabla \quad (27.28)$$

$$\text{classical Hamiltonian of the electron: } \mathbf{H} = \frac{\mathbf{p}^2}{2 \cdot m} + \frac{\mathbf{A}^2 \cdot q_e^2}{2 \cdot c^2 \cdot m} + \frac{\mathbf{A} \cdot \mathbf{p} \cdot q_e}{c \cdot m} - q_e \cdot V(\mathbf{r}) + \Theta(\mathbf{r}) \quad (27.29)$$

$$\text{QM Hamiltonian operator } \mathbf{H} = \frac{\hbar^2}{2 \cdot m} \cdot \nabla^2 + \frac{i \cdot q_e \cdot \hbar}{2 \cdot m \cdot c} \cdot (\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla) + \frac{q_e^2}{2 \cdot m \cdot c^2} \cdot \mathbf{A}^2 - q_e \cdot V + \Theta \quad (27.30)$$

► H+H^†

$$\text{Probability current density } \mathbf{J} = \frac{\hbar}{2 \cdot m \cdot i} \cdot \left( \psi^* \cdot \nabla \Psi - \Psi \cdot \nabla \psi^* - 2i \cdot \frac{q_e}{\hbar \cdot c} \cdot \mathbf{A} \cdot \psi^* \cdot \Psi \right) \quad (27.31)$$

$$\text{or } \mathbf{J} = \frac{\hbar}{2 \cdot m \cdot i} \cdot \left( \psi^* \cdot \nabla \Psi - \Psi \cdot \nabla \psi^* - \frac{q_e}{m \cdot c} \cdot \psi^* \cdot \Psi \cdot \mathbf{A} \right) \quad (27.32)$$

▼

One-dimensional Schrödinger equation in absence of potentials:  $V = 0$  volt, and  $\Theta = 0$  J.

$$\text{Schrödinger equation } \frac{\hbar^2}{2 \cdot m} \cdot \frac{\partial^2}{\partial x^2} \Psi = \frac{\hbar}{i} \cdot \frac{\partial}{\partial t} \Psi \quad (27.33)$$

$$\text{Eigenfunction } \Psi(k, x, t) = \alpha \cdot e^{i \cdot (k \cdot x - \omega \cdot t)} + \beta \cdot e^{-i \cdot (k \cdot x + \omega \cdot t)} = C(k) \cdot e^{i \cdot (k \cdot x - \omega \cdot t)} \quad (27.34)$$

$$\psi(x, t) = \int_{-\infty}^{\infty} \Psi(k, x, t) dk \quad (27.35)$$

$$\text{For } t = 0 \cdot s \quad \psi(x, 0) = \alpha \cdot e^{\frac{-x^2}{2 \cdot a^2} + i \cdot k_0 \cdot x} \quad p_0 = \hbar \cdot k_0$$

$$\rho(x, 0) = \psi^* \cdot \psi = \left( \alpha \cdot e^{\frac{-x^2}{2 \cdot a^2} + i \cdot k_0 \cdot x} \right)^* \cdot \left( \alpha \cdot e^{\frac{-x^2}{2 \cdot a^2} + i \cdot k_0 \cdot x} \right) = (|\alpha|)^2 \cdot e^{\frac{-x^2}{a^2}}$$

$$\int_{-\infty}^{\infty} \rho(x, 0) dx = 1 \quad (|\alpha|)^2 = \frac{1}{a \cdot \sqrt{\pi}}$$

$$S(x, 0) = \rho \cdot \frac{\hbar}{m} \cdot k_0$$

$$\Psi(x, 0) = \int_{-\infty}^{\infty} C(k) \cdot e^{i \cdot k \cdot x} dk$$

$$C(k) = \frac{1}{2 \cdot \pi} \cdot \int_{-\infty}^{\infty} \Psi(x, 0) \cdot e^{-i \cdot k \cdot x} dx = \frac{\alpha \cdot a}{\sqrt{2 \cdot \pi}} \cdot e^{\frac{-1}{2} \cdot a^2 \cdot (k - k_0)^2}$$

$$\Psi(x, t) = \frac{\alpha}{\sqrt{1 + i \cdot \frac{\hbar \cdot t}{m \cdot a^2}}} \cdot e^{\frac{x^2 - i \cdot a^2 \cdot k_0 \cdot \left( 2 \cdot x - \frac{\hbar \cdot t}{2 \cdot m} \cdot k_0 \right)}{2 \cdot a^2 \cdot \left( 1 + i \cdot \frac{\hbar \cdot t}{m \cdot a^2} \right)}} \quad (27.36)$$

►

► varie

Remark on parity [4]

$$\left( \frac{-\hbar^2}{2 \cdot m} \cdot \Delta + V(x) \right) | \psi \rangle = E | \psi \rangle$$

$$V(x) = \frac{\hbar^2}{2 \cdot m} \cdot U(x) \quad E = \frac{\hbar^2}{2 \cdot m} \cdot \epsilon$$

$$\left( \frac{-\hbar^2}{2 \cdot m} \cdot \Delta + \frac{\hbar^2}{2 \cdot m} \cdot U(x) \right) | \psi \rangle = \frac{\hbar^2}{2 \cdot m} \cdot \epsilon | \psi \rangle$$

$$(-\Delta + U(x)) | \psi \rangle = \epsilon | \psi \rangle$$

$$\Delta | \psi \rangle = (U - \epsilon) | \psi \rangle$$

$$\frac{\partial^2}{\partial x^2} \psi(x) - (U - \epsilon) \cdot \psi(x) = 0$$

If the potential U is even, that is to say if  $U(x) = U(-x)$ , the Schrödinger Hamiltonian doesn't change when I replace x with -x, that is it is *invariant under reflection through the origin*. It follows that if  $\psi(x)$  is an eigenfunction of the eigenvalue E, equation changes as follows:

$$\mathbf{H} | \psi(x) \rangle = E | \psi(x) \rangle \quad \rightarrow \quad \mathbf{H} | \psi(-x) \rangle = E | \psi(-x) \rangle$$

The even function  $\psi(x) + \psi(-x)$  and the odd function  $\psi(x) - \psi(-x)$  are both eigenfunctions of the same eigenvalue E and at least one does vanish identically.

1) **E is not degenerate**, then the four functions ( $\psi(x)$ ,  $\psi(-x)$ ,  $\psi(x) + \psi(-x)$ ,  $\psi(x) - \psi(-x)$ ) are multiples of each other.  $\psi(x)$  is a multiple of the one not identically zero.

The eigenfunction of a non degenerate eigenvalue (spectrum) some are even and the other are odd. The ground state is always even. Increasing the eigenvalues of the energy, alternately the eigenfunctions are even and odd.

2) **E is degenerate**, then each eigenfunction  $\psi$  is a linear combination of the linear and independent function f, g each having its parity: for example  $\psi(x) = \lambda f(x) + \mu g(x)$ . The eigenvalues of the continuous spectrum are all doubly degenerate and to each of the corresponds an even function and an odd.

If the Hamiltonian of the system is invariant under certain transformations, the eigenfunctions have certain symmetry properties. Parity is an example of this.

Consider the observable parity indicated with **P**:

$$\mathbf{P} | \psi(x) \rangle = | \psi(-x) \rangle,$$

P is Hermitian

$$\mathbf{P} = \mathbf{P}^\dagger,$$

$$\mathbf{P}^2 = 1.$$

The eigenvalues  $\lambda$  of  $\mathbf{P} | \psi(q) \rangle = \lambda | \psi(-q) \rangle$  are necessarily  $\lambda_1 = 1$  and  $\lambda_2 = -1$ .

The eigenfunction associated with the eigenvalue  $\lambda_1 = 1$  are even,

while the eigenfunction associated with the eigenvalue  $\lambda_2 = -1$  are odd.

When the Schrödinger Hamiltonian is *invariant under reflection through the origin*, results:

$$[\mathbf{P}, \mathbf{H}] = 0.$$

$$\text{If } \mathbf{H} \left( \frac{\hbar}{i} \cdot \frac{d}{dq}, q \right) = \mathbf{H} \left( -\frac{\hbar}{i} \cdot \frac{d}{dq}, -q \right) \Rightarrow \forall | \psi(q) \rangle,$$

$$\mathbf{P} \mathbf{H} | \psi(q) \rangle = \mathbf{H} \left( -\frac{\hbar}{i} \cdot \frac{d}{dq}, -q \right) | \psi(-q) \rangle = \mathbf{H} \left( \frac{\hbar}{i} \cdot \frac{d}{dq}, q \right) | \psi(q) \rangle = \mathbf{H} \mathbf{P} | \psi(q) \rangle.$$

For  $t=0$  and the same condition, if the wave function has a definite parity, it conserves the same parity in the course of time.

$$\text{Hermitian} \quad \sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (28.1)$$

$$\text{Anti Hermitian} \quad i \cdot \sigma_1 = \begin{pmatrix} 0 & j \\ j & 0 \end{pmatrix} \quad i \cdot \sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad i \cdot \sigma_3 = \begin{pmatrix} j & 0 \\ 0 & -j \end{pmatrix} \quad (28.2)$$

Calculations

**Statistical mixture of states:** the dynamical state of the system is *incompletely known*. One assigns to the system a statistical mixture of wave functions each having a suitable statistical weight.

Methods to study incompletely known dynamical states of a quantum system.

When information regarding a system is incomplete, I simply state that the system has some probabilities  $p_1, p_2, \dots, p_n$  to find itself in the dynamical states represented by the ket vectors  $|1\rangle, |2\rangle, \dots, |n\rangle$ . In other words the dynamical state of the system can't be represented by a single vector but by a statistical mixture of vectors.

Suppose I perform the measurement of the physical quantity  $A$ ; it is an observable so that it is represented by the operator  $\hat{A}$ . After  $n$  measurements I have the average value of the  $n$  results indicated with  $\langle A \rangle_n$ .

$$\langle A \rangle_n = \frac{(\langle n | \hat{A} | n \rangle)}{\langle n | n \rangle} \quad (29.1)$$

For normalized eigenvectors I have  $\langle n | n \rangle = 1$ , so that:  $\langle A \rangle_n = \langle n | \hat{A} | n \rangle$ , while

$$\langle A \rangle = \sum_n [p_n \cdot (\langle A \rangle_n)] = \sum_n (p_n \cdot \langle n | \hat{A} | n \rangle) \quad (29.2)$$

in fact if I indicate with  $a_{ij}$  the result of each measurement, I have:  $\langle A \rangle_i = \frac{j}{n_i} = \langle i | \hat{A} | i \rangle$  with  $\langle i | i \rangle = 1$

$$\langle A \rangle = \frac{\sum_i \sum_j a_{ij}}{\sum_k n_k} = \frac{\sum_i [n_i \cdot (\langle A \rangle_i)]}{\sum_k n_k} = \sum_i \left[ \frac{n_i}{\sum_k n_k} \cdot (\langle A \rangle_i) \right] \quad (29.3)$$

$$\text{define the statistical weight as: } \frac{n_i}{\sum_k n_k} = p_i \quad (29.4)$$

$$\text{so that } \langle A \rangle = \sum_n [p_n \cdot (\langle A \rangle_n)] = \sum_n (p_n \cdot \langle n | \hat{A} | n \rangle) \quad (29.5)$$

$$\text{the statistical weight is given by the projector: } \mathbf{P}_n = |n\rangle \langle n| \quad p_n \geq 0 \quad \sum_n p_n = 1 \quad (29.6)$$

$$\mathbf{P} = \sum_n \mathbf{P}_n = \sum_n |n\rangle \langle n| \quad (29.7)$$

$$\text{Consider the projector } \mathbf{P}_n = |n\rangle \langle n| \quad \text{Tr}(\mathbf{P}_n) = 1$$

$$\text{Tr}(\mathbf{P}_n \cdot \mathbf{A}) = \text{Tr}(\mathbf{P}_n^2 \cdot \mathbf{A}) = \text{Tr}(\mathbf{P}_n \cdot \mathbf{A} \cdot \mathbf{P}_n)$$

$$\text{Tr}(\mathbf{P}_n \cdot \mathbf{A} \cdot \mathbf{P}_n) = \text{Tr}(|n\rangle \langle n| \cdot \mathbf{A} \cdot |n\rangle \langle n|) = \langle n | \hat{A} | n \rangle \cdot \text{Tr}(|n\rangle \langle n|) = \langle n | \hat{A} | n \rangle$$

$$\text{If } \mathbf{A}=1 \quad \text{Tr}(\mathbf{P}_n) = \langle n | n \rangle = 1$$

$$\langle \mathbf{A} \rangle = \sum_n [p_n \cdot (\langle \mathbf{A} \rangle_n)] = \sum_n (p_n \cdot \langle n | \mathbf{A} | n \rangle) = \sum_n (p_n \cdot \text{Tr}(\mathbf{P}_n \cdot \mathbf{A})) = \sum_n (p_n \cdot \text{Tr}(|n\rangle \langle n| \cdot \mathbf{A}))$$

**Statistic Operator or Density Operator:**  $\rho = \sum_n |n\rangle p_n \langle n| \quad \langle n | n \rangle = 1$  (29.8)

Knowing  $\rho$ , I can find the statistical distribution of the results of measurement of  $\mathbf{A}$

The dynamical state of the system is represented usefully by the statistical mixture of ket vectors.

$p_n$  is a statistical weight  $\sum_n p_n = 1$  (29.9)

$$\rho > 0$$
 (29.10)

$$\rho = \rho^\dagger$$
 (29.11)

$$\text{Tr}(\rho \cdot \mathbf{A}) = \langle \mathbf{A} \rangle \quad \mathbf{A} = 1 \quad \text{Tr}(\rho) = 1$$

Operator trace  $\text{Tr}(\rho) = 1$  (29.12)

$$\text{Tr}(\rho^2) \leq 1$$
 (29.13)

Average value of the observable  $\mathbf{A}$ :  $\langle \mathbf{A} \rangle = \text{Tr}(\rho \cdot \mathbf{A}) = \langle n | \mathbf{A} | n \rangle$  (29.14)

Average value of the function of the observable  $F(\mathbf{A})$ :  $\langle F(\mathbf{A}) \rangle = \text{Tr}(\rho \cdot F(\mathbf{A}))$  (29.15)

The probability that the result of measurement belong to domain  $D$  of the spectrum of  $\mathbf{A}$  is

$$w_D = \langle \mathbf{P}_D \rangle = \text{Tr}(\rho \cdot \mathbf{P}_D),$$

(29.16)

where  $\mathbf{P}_D$  is the projector upon the subspace spanned by the eigenvectors of  $\mathbf{A}$ .

The probability of finding the system in the quantum state represented by the normalize ket  $|x\rangle$ , is:

$$w_x = \text{Tr}(\rho \cdot |x\rangle \langle x|)$$
 (29.17)

Two statistical mixtures possessing the same density operator, are identical.

**The Schrödinger equation of the Density Operator:**

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} \rho = [ \mathbf{H}, \rho ]$$
 (29.18)

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} \rho_{k,1} = \langle k | [ \mathbf{H}, \rho ] | 1 \rangle$$
 (29.19)

$$\mathbf{H} = \mathbf{H}^\dagger \Rightarrow \frac{\partial}{\partial t} \rho_{k,1} = -i \cdot \omega_{k,1} \cdot \rho_{k,1}$$
 (29.20)

$$\omega_{k,1} = \frac{E_k - E_1}{\hbar}$$
 (29.21)

$$\rho(t)_{k,1} = \rho(0)_{k,1} \cdot e^{-i \cdot \omega_{k,1} \cdot (t-t_0)}$$
 (29.22)

$$\text{for } k=1 \quad \omega_{k,k} = \frac{E_k - E_k}{\hbar} = 0 \quad \rho_{k,k} = \rho_{k,k}(0) \quad \text{all elements of the diagonal are unchanged}$$

**Pure state:** when the dynamical state of the system is *exactly known* one says that "one is dealing with a *pure state*". The pure state  $|\chi\rangle$  can be represented as the only state of a statistical mixture; so that its density operator is:

$$\rho_\chi = |\chi\rangle \langle \chi|$$

$$\rho_\chi^2 = \rho_\chi$$

If a density operator is a projector, than it represents a pure state.

Since a density operator can be represented by the superposition:

$$\rho = \sum_n |n\rangle p_n \langle n|,$$

in order that it represents a pure state it is necessary and sufficient that each  $|n\rangle$  be equal to each other to within a

phase. Furthermore if  $\text{Tr}(\rho^2) = 1$ , than the density operator represents a pure state.

The state of a quantum system whose Hamiltonian is  $\mathbf{H}$ , in thermodynamic equilibrium at temperature  $T$  is represented by the operator

$$\rho = N \cdot e^{-\frac{\mathbf{H}}{k_B T}},$$

where  $k_B$  is the Boltzmann constant and  $N$  is a normalization constant such that  $\text{Tr}(\rho)=1$ .

System entropy:

$$S = -k_B \cdot \text{Tr}(\rho \cdot \ln(\rho))$$

### 30 Hamiltonian for macroscopic systems and small interactions close to equilibrium

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_{\text{int}} + \mathbf{H}_r \quad (30.1)$$

Unperturbed Hamiltonian  $\mathbf{H}_0$   
 Interaction Hamiltonian  $\mathbf{H}_{\text{int}}$   
 Relaxation Hamiltonian  $\mathbf{H}_r$

$$i\hbar \frac{\partial}{\partial t} \rho_{k,j} = ([\mathbf{H}_0, \rho])_{k,j} + ([\mathbf{H}_{\text{int}}, \rho])_{k,j} + ([\mathbf{H}_r, \rho])_{k,j}$$

$$\mathbf{H}_0 > \mathbf{H}_{\text{int}} \wedge \mathbf{H}_0 > \mathbf{H}_r \Rightarrow -i\hbar \frac{\partial}{\partial t} \rho_{k,j} = ([\mathbf{H}_r, \rho])_{k,j} \quad k \neq j$$

$$\mathbf{H}_1 = \mathbf{H}_0 + \mathbf{H}_{\text{int}}$$

$$\begin{pmatrix} i\hbar \frac{\partial}{\partial t} \rho_{k,j} \\ i\hbar \frac{\partial}{\partial t} \rho_{k,j} \end{pmatrix} = \begin{bmatrix} i\hbar \frac{\rho_{k,j}}{\tau_{k,j}} \\ ([\mathbf{H}_1, \rho])_{k,j} + i\frac{\hbar}{T_1} (\rho_{e_{k,k}} - \rho_{k,k}) \end{bmatrix}$$

If  $\mathbf{H}_{\text{int}} = 0 \Rightarrow ([\mathbf{H}_0, \rho])_{k,k} = C_0 \Rightarrow W_{n,k} \rho_{e_{n,n}} = W_{k,n} \rho_{e_{k,k}}$  *this is the "detailed balance principle"*

### 31 Algebra of the one-dimensional harmonic oscillator [7]

The classical Hamiltonian of a simple (without damping) mechanical oscillator (composed by a mass m) is:

$$\mathbf{H} = \frac{1}{2} m \cdot x'^2 + \frac{m \cdot \omega^2}{2} \cdot x^2 \quad (31.1)$$

considering the Lagrangian conjugated momenta, I can write:  $\mathbf{H} = \frac{1}{2} m \cdot q'^2 + \frac{1}{2} m \cdot \omega^2 \cdot q^2$  (31.1)

where:  $x' = q'$   $p = m \cdot q'$   $q'^2 = \left(\frac{p}{m}\right)^2 = \frac{p^2}{m^2}$  (31.2)

so that the Hamiltonian takes the form:  $\mathbf{H} = \frac{1}{2 \cdot m} \cdot (p^2 + m^2 \cdot \omega^2 \cdot q^2)$  (31.3)

Quantization rules (when the quantum system possesses a classical analogue)

Classical Operator	Quantized Operator acting on kets or eigenfunctions
$\mathbf{p}$	$\leftrightarrow -i \cdot \hbar \cdot \nabla$
$\mathbf{q}'$	$\leftrightarrow -i \cdot \frac{\hbar}{m} \cdot \nabla$
$\mathbf{p}^2$	$\leftrightarrow -\hbar^2 \cdot \Delta$
$\frac{\mathbf{p} \cdot \mathbf{q}'}{2} = \frac{\mathbf{p}^2}{2 \cdot m}$	$\leftrightarrow \frac{-\hbar^2}{2 \cdot m} \cdot \Delta$
Energy E	$\leftrightarrow i \cdot \hbar \cdot \frac{\partial}{\partial t}$

It follows that:  $\mathbf{H} = \frac{1}{2 \cdot m} \cdot (p^2 + m^2 \cdot \omega^2 \cdot q^2) \leftrightarrow \mathbf{H} = \frac{-\hbar^2}{2 \cdot m} \cdot \Delta + \frac{m \cdot \omega^2}{2} \cdot q^2$  (31.4)

The Schrödinger equation of motion is:

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \mathbf{H} |\Psi\rangle \quad (31.5)$$

that is:  $i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \left( \frac{-\hbar^2}{2 \cdot m} \cdot \Delta + \frac{m \cdot \omega_0^2}{2} \cdot q^2 \right) |\Psi\rangle$  (31.6)

When the system is in a stationary state of energy E, I get:  $|\Psi\rangle = e^{-i \frac{E \cdot t}{\hbar}} |\psi\rangle$

$$E |\psi\rangle = \mathbf{H} |\psi\rangle$$

Commutator [q,p] calculations

with the previous assumption I want see how the Hamiltonia  $\mathbf{H}$  is related to the Lagrangian variables position  $\mathbf{q}$  and conjugated momentum  $\mathbf{p}$ . I found that:

$$[\mathbf{q}, \mathbf{p}] = i \cdot \hbar \quad (31.7)$$

Define the new operators:  $\mathbf{q} = \sqrt{\frac{\hbar}{m \cdot \omega}} \cdot \mathbf{Q}$  and  $\mathbf{p} = \sqrt{\hbar \cdot m \cdot \omega} \cdot \mathbf{P}$  [7] (31.8)

substituting in (31.7) I get:

$$[\mathbf{q}, \mathbf{p}] = \mathbf{q} \cdot \mathbf{p} - \mathbf{p} \cdot \mathbf{q} = \sqrt{\frac{\hbar}{m \cdot \omega}} \cdot \mathbf{Q} \cdot \sqrt{\hbar \cdot m \cdot \omega} \cdot \mathbf{P} - \sqrt{\hbar \cdot m \cdot \omega} \cdot \mathbf{P} \cdot \sqrt{\frac{\hbar}{m \cdot \omega}} \cdot \mathbf{Q} = \hbar \cdot (\mathbf{Q} \cdot \mathbf{P} - \mathbf{P} \cdot \mathbf{Q}) = \hbar \cdot ([\mathbf{Q}, \mathbf{P}]) = i \cdot \hbar$$

it follows necessarily, that  $[\mathbf{Q}, \mathbf{P}] = i \cdot \mathbf{I}$  (31.9)

Furthermore substituting (31.8) into the Hamiltonian (31.4), results:

$$\mathbf{H} = \frac{1}{2 \cdot m} \cdot (\mathbf{p}^2 + m^2 \cdot \omega^2 \cdot \mathbf{q}^2) = \frac{1}{2 \cdot m} \cdot \left( \hbar \cdot m \cdot \omega \cdot \mathbf{P}^2 + m^2 \cdot \omega^2 \cdot \frac{\hbar}{m \cdot \omega} \cdot \mathbf{Q}^2 \right)$$

$$\mathbf{H} = \frac{1}{2 \cdot m} \cdot (\hbar \cdot m \cdot \omega \cdot \mathbf{P}^2 + \hbar \cdot m \cdot \omega \cdot \mathbf{Q}^2) = \frac{\hbar \cdot \omega}{2} \cdot (\mathbf{P}^2 + \mathbf{Q}^2) \quad (31.10)$$

namely:  $\mathbf{H} = \frac{\hbar \cdot \omega}{2} \cdot (\mathbf{P}^2 + \mathbf{Q}^2)$  (31.11)

I place:  $\mathbf{H} = \hbar \cdot \omega \cdot \mathbf{H}_0$

so that, thanks to (31.11), I get:  $\mathbf{H}_0 = \frac{1}{2} \cdot (\mathbf{P}^2 + \mathbf{Q}^2)$  (31.12)

☐ (Q+iP)(Q-iP)

$$(\mathbf{Q} + i \cdot \mathbf{P}) \cdot (\mathbf{Q}_1 - i \cdot \mathbf{P}_1) = \mathbf{Q} \cdot \mathbf{Q}_1 - i \cdot \mathbf{Q} \cdot \mathbf{P}_1 + i \cdot \mathbf{P} \cdot \mathbf{Q}_1 + \mathbf{P} \cdot \mathbf{P}_1 = \mathbf{Q} \cdot \mathbf{Q}_1 + \mathbf{P} \cdot \mathbf{P}_1 - i \cdot (\mathbf{Q} \cdot \mathbf{P}_1 - \mathbf{P} \cdot \mathbf{Q}_1)$$

$$(\mathbf{Q} + i \cdot \mathbf{P}) \cdot (\mathbf{Q} - i \cdot \mathbf{P}) = \mathbf{Q} \cdot \mathbf{Q} - i \cdot \mathbf{Q} \cdot \mathbf{P} + i \cdot \mathbf{P} \cdot \mathbf{Q} + \mathbf{P} \cdot \mathbf{P} = \mathbf{Q}^2 + \mathbf{P}^2 - i \cdot (\mathbf{Q} \cdot \mathbf{P} - \mathbf{P} \cdot \mathbf{Q}) = \mathbf{Q}^2 + \mathbf{P}^2 + \mathbf{I}$$

since from (31.9):  $[\mathbf{Q}, \mathbf{P}] = i \cdot \mathbf{I}$

$$(\mathbf{Q} + i \cdot \mathbf{P}) \cdot (\mathbf{Q} - i \cdot \mathbf{P}) = \mathbf{Q}^2 + \mathbf{P}^2 + \mathbf{I}$$

☐ (Q+iP)(Q-iP)

☐ (Q-iP)(Q+iP)

$$(\mathbf{Q} - i \cdot \mathbf{P}) \cdot (\mathbf{Q}_1 + i \cdot \mathbf{P}_1) = \mathbf{Q} \cdot \mathbf{Q}_1 + i \cdot \mathbf{Q} \cdot \mathbf{P}_1 - i \cdot \mathbf{P} \cdot \mathbf{Q}_1 + \mathbf{P} \cdot \mathbf{P}_1 = \mathbf{Q} \cdot \mathbf{Q}_1 + \mathbf{P} \cdot \mathbf{P}_1 + i \cdot (\mathbf{Q} \cdot \mathbf{P}_1 - \mathbf{P} \cdot \mathbf{Q}_1)$$

$$(\mathbf{Q} - i \cdot \mathbf{P}) \cdot (\mathbf{Q} + i \cdot \mathbf{P}) = \mathbf{Q} \cdot \mathbf{Q} + i \cdot \mathbf{Q} \cdot \mathbf{P} - i \cdot \mathbf{P} \cdot \mathbf{Q} + \mathbf{P} \cdot \mathbf{P} = \mathbf{Q}^2 + \mathbf{P}^2 + i \cdot (\mathbf{Q} \cdot \mathbf{P} - \mathbf{P} \cdot \mathbf{Q})$$

thanks to (31.9) I get:  $(\mathbf{Q} - i \cdot \mathbf{P}) \cdot (\mathbf{Q} + i \cdot \mathbf{P}) = \mathbf{Q}^2 + \mathbf{P}^2 - \mathbf{I}$

☐ (Q-iP)(Q+iP)

Since I deal with vectorial operators I have:

$$\mathbf{P}^2 + \mathbf{Q}^2 = (\mathbf{Q} + i \cdot \mathbf{P}) \cdot (\mathbf{Q} - i \cdot \mathbf{P}) - \mathbf{I}$$

the Hamiltonian (31.12) can be rewritten as:  $\mathbf{H}_0 = \frac{1}{2} \cdot [(\mathbf{Q} + i \cdot \mathbf{P}) \cdot (\mathbf{Q} - i \cdot \mathbf{P}) - \mathbf{I}]$

A further simplification is reached with defining the three new following QM operators:

(Ladder) operator:  $\mathbf{a} = \frac{1}{\sqrt{2}} \cdot (\mathbf{Q} + i \cdot \mathbf{P})$  (31.13)

(Ladder) operator:  $\mathbf{a}^\dagger = \frac{1}{\sqrt{2}} \cdot (\mathbf{Q} - i \cdot \mathbf{P})$  (31.14)

Since  $\mathbf{a} \neq \mathbf{a}^\dagger$  they aren't Hermitian.

Number operator:  $\mathbf{N} = \mathbf{a}^\dagger \cdot \mathbf{a}$   $\mathbf{N}^\dagger = \mathbf{a} \cdot \mathbf{a}^\dagger$  (31.15)

Complex conjugated of  $\mathbf{a}$ :  $\mathbf{a}^* = \frac{1}{\sqrt{2}} \cdot (\mathbf{Q} + i \cdot \mathbf{P})^* = \frac{1}{\sqrt{2}} \cdot (\mathbf{Q} - i \cdot \mathbf{P}) = \mathbf{a}^\dagger$

adjoint or Hermitian conjugate:  $\mathbf{a}^* = \mathbf{a}^\dagger$

other noteworthy relations between  $\mathbf{a}$  and  $\mathbf{a}^\dagger$  are:

the sum:  $\mathbf{a}^\dagger + \mathbf{a} = \frac{1}{\sqrt{2}} \cdot (\mathbf{Q} - i \cdot \mathbf{P} + \mathbf{Q} + i \cdot \mathbf{P}) = \sqrt{2} \cdot \mathbf{Q}$  (31.16)

$$\mathbf{Q} = \frac{1}{\sqrt{2}} \cdot (\mathbf{a}^\dagger + \mathbf{a}) \quad (31.17)$$

the difference:  $\mathbf{a}^\dagger - \mathbf{a} = \frac{1}{\sqrt{2}} \cdot [\mathbf{Q} - i \cdot \mathbf{P} - (\mathbf{Q} + i \cdot \mathbf{P})] = \sqrt{2} \cdot i \cdot \mathbf{P}$  (31.18)

$$\mathbf{P} = \frac{1}{\sqrt{2}} \cdot (\mathbf{a}^\dagger - \mathbf{a}) \quad (31.19)$$

Product:  $\mathbf{a} \cdot \mathbf{a}^\dagger = \frac{1}{2} \cdot (\mathbf{Q} + i \cdot \mathbf{P}) \cdot (\mathbf{Q} - i \cdot \mathbf{P}) = \frac{1}{2} \cdot (\mathbf{P}^2 + \mathbf{Q}^2 + \mathbf{I}) = \mathbf{H}_0 + \frac{1}{2} \cdot \mathbf{I}$  (31.20)

$\mathbf{a}^\dagger \cdot \mathbf{a} = \frac{1}{2} \cdot (\mathbf{Q} - i \cdot \mathbf{P}) \cdot (\mathbf{Q} + i \cdot \mathbf{P}) = \frac{1}{2} \cdot (\mathbf{Q}^2 + \mathbf{P}^2 - \mathbf{I}) = \mathbf{H}_0 - \frac{1}{2} \cdot \mathbf{I}$  (31.21)

The commutator between  $\mathbf{a}$  and  $\mathbf{a}^\dagger$  can be found using (31.20) and (31.21):

$$[\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{a} \cdot \mathbf{a}^\dagger - \mathbf{a}^\dagger \cdot \mathbf{a} = \mathbf{H}_0 + \frac{1}{2} \cdot \mathbf{I} - \left( \mathbf{H}_0 - \frac{1}{2} \cdot \mathbf{I} \right) = \mathbf{I}$$

$$[\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{I} \quad [\mathbf{a}^\dagger, \mathbf{a}] = -\mathbf{I} \quad (31.22)$$

From (31.21) I get the operator number as a function of the Hamiltonian  $\mathbf{H}$ :

$$\mathbf{N} = \mathbf{a}^\dagger \cdot \mathbf{a} = \mathbf{H}_0 - \frac{1}{2} \cdot \mathbf{I} \quad (31.23)$$

that is the Hamiltonian takes the form:  $\mathbf{H}_0 = \mathbf{N} + \frac{1}{2} \cdot \mathbf{I}$   $\mathbf{H} = \hbar \cdot \omega \cdot \mathbf{H}_0$  (31.24)

The Hamiltonian can also take other forms, in fact consider the commutator:

$$[\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{a} \cdot \mathbf{a}^\dagger - \mathbf{a}^\dagger \cdot \mathbf{a} = \mathbf{N}^\dagger - \mathbf{N} \quad (31.25)$$

From (31.20), I have:  $\mathbf{N}^\dagger = \mathbf{a} \cdot \mathbf{a}^\dagger = \mathbf{H}_0 + \frac{1}{2} \cdot \mathbf{I}$  (31.26)

namely:  $\mathbf{N}^\dagger = \mathbf{H}_0 + \frac{1}{2} \cdot \mathbf{I}$  (31.27)



Calculation of the commutator  $[N, a] = [a^\dagger \cdot a, a] = a^\dagger \cdot a \cdot a - a \cdot a^\dagger \cdot a$        $a^\dagger \cdot a = a \cdot a^\dagger - I$

□  $[N, a]$  —————  
 the result is:  $[N, a] = -a$  (31.28)

I adopt the same procedure to calculate the commutator  $[N, a^\dagger]$ , namely:  $a \cdot a^\dagger = a^\dagger \cdot a + I$

□  $[N, a^\dagger]$  —————  
 the result is:  $[N, a^\dagger] = a^\dagger$  (31.29)

Can be useful to calculate the following difference using (31.27) and (31.24):

$$N^\dagger - N = a \cdot a^\dagger - a^\dagger \cdot a = H_0 + \frac{1}{2} \cdot I - H_0 + \frac{1}{2} \cdot I = I$$

$$N = N^\dagger - I$$

$$N^\dagger = N + I$$

$$N^\dagger - N = I$$

The sum:  $N^\dagger + N = H_0 + \frac{1}{2} \cdot I + H_0 - \frac{1}{2} \cdot I = 2 \cdot H_0$

$$H_0 = \frac{1}{2} \cdot (N^\dagger + N)$$
 (31.30)

The Hamiltonian as a function of  $a$  and  $a^\dagger$ :

from (31.28):  $H_0 = \frac{1}{2} \cdot (N^\dagger + N) = \frac{1}{2} \cdot (a^\dagger \cdot a + a \cdot a^\dagger)$  (31.31)

from (31.27) I get:  $H_0 = N^\dagger - \frac{1}{2} \cdot I$        $H = \hbar \cdot \omega \cdot H_0$  (31.32)

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} | \psi \rangle = H_0 | \psi \rangle = \left( N^\dagger - \frac{1}{2} \cdot I \right) | \psi \rangle$$

The *Schrödinger equation* of motion is:  $\frac{\partial}{\partial t} | \psi \rangle = \frac{-i}{\hbar} \cdot \left( N^\dagger - \frac{1}{2} \cdot I \right) | \psi \rangle$  (31.33)

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} | \psi \rangle = H_0 | \psi \rangle = \left( N + \frac{1}{2} \cdot I \right) | \psi \rangle$$

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} | \psi \rangle = \left( N + \frac{1}{2} \cdot I \right) | \psi \rangle$$

The *Schrödinger equation* of motion is:  $\frac{\partial}{\partial t} | \psi \rangle = \frac{-i}{\hbar} \cdot \left( N + \frac{1}{2} \cdot I \right) | \psi \rangle$  (31.34)

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} | \psi \rangle = H_0 | \psi \rangle = \frac{1}{2} \cdot (a \cdot a^\dagger + a^\dagger \cdot a) | \psi \rangle$$

The *Schrödinger equation* of motion is:  $\frac{\partial}{\partial t} | \psi \rangle = \frac{-i}{2 \cdot \hbar} \cdot (a^\dagger \cdot a + a \cdot a^\dagger) | \psi \rangle$  (31.35)

### 32 Eigenvalues and eigenvectors of the energy associated with $H$ and $N$ [7]

Assuming that there exists at least one eigenket of  $N$  in Hilbert space  $\mathbb{H}$ , I can write:

$$N | \varphi_\nu \rangle = \nu | \varphi_\nu \rangle, \quad (32.1)$$

where  $N = a^\dagger \cdot a$  and  $\langle \varphi_\nu | \varphi_\nu \rangle = \lambda_\nu$ , that is the ket  $| \varphi_\nu \rangle$  isn't normalized.

Now write the eigenvalue equation for the ket:  $a | \varphi_\nu \rangle$  keeping in mind (32.28)  $[N, a] = -a$  (32.2)

$$[N, a] = N \cdot a - a \cdot N \quad N \cdot a = [N, a] + a \cdot N = -a + a \cdot N = a \cdot (N - I)$$

$$N \cdot a | \varphi_\nu \rangle = a \cdot (N - I) | \varphi_\nu \rangle = (\nu - 1) \cdot a | \varphi_\nu \rangle, \quad (32.3)$$

□

Knowing that [eq. (32.22)]:  $[a, a^\dagger] = a \cdot a^\dagger - a^\dagger \cdot a = I$

it follows that:  $a^\dagger \cdot a = a \cdot a^\dagger - I$  (32.4)

apply  $a$  on the right of (32.4):  $a^\dagger \cdot a \cdot a = (a \cdot a^\dagger - I) \cdot a = a \cdot a^\dagger \cdot a - a = a \cdot (a^\dagger \cdot a - I)$  (32.5)

so that eq. (32.3) can be rewritten as:  $N \cdot a | \varphi_\nu \rangle = a^\dagger \cdot a \cdot a | \varphi_\nu \rangle = (a \cdot a^\dagger - I) \cdot a | \varphi_\nu \rangle$

therefore:  $N \cdot a | \varphi_\nu \rangle = a \cdot (a^\dagger \cdot a - I) | \varphi_\nu \rangle = a \cdot (N - I) | \varphi_\nu \rangle$

resulting:  $N \cdot a = a \cdot (N - I)$  (32.6)

the eigenvalues equation is:  $a \cdot (N - I) | \varphi_\nu \rangle = a \cdot (\nu - 1) | \varphi_\nu \rangle = (\nu - 1) \cdot a | \varphi_\nu \rangle$

finally resulting:  $N \cdot a | \varphi_\nu \rangle = (\nu - 1) \cdot a | \varphi_\nu \rangle$  (32.7)

□

The ket:  $a | \varphi_\nu \rangle$  is an eigenvector of  $N$  with eigenvalue  $\nu - 1$ . I can define the new eigenvector:

$$C | \varphi_{\nu-1} \rangle = a | \varphi_\nu \rangle$$

the equation (32.7) become:  $N \cdot C | \varphi_{\nu-1} \rangle = (\nu - 1) \cdot C | \varphi_{\nu-1} \rangle$

namely:  $N | \varphi_{\nu-1} \rangle = (\nu - 1) | \varphi_{\nu-1} \rangle$  (32.8)

With the same procedure I define the ket:  $C | \varphi_{\nu-2} \rangle = a | \varphi_{\nu-1} \rangle = a \cdot (a | \varphi_\nu \rangle) = a^2 | \varphi_\nu \rangle$

and so on, finding the  $m^{\text{th}}$  eigenvector of  $N$  as:  $| \varphi_{\nu-m} \rangle = a^m | \varphi_\nu \rangle$  (32.9)

Now write the eigenvalue equation (32.1) for the ket:  $a^\dagger | \varphi_\nu \rangle$  that is:  $N \cdot a^\dagger | \varphi_\nu \rangle = a^\dagger | \varphi_\nu \rangle$ ,

since:  $N = a^\dagger \cdot a$ ,

$$\text{the eigenvalues equation takes the form: } \mathbf{N} \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle = \mathbf{a}^\dagger \cdot \mathbf{a} \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle \quad (32.10)$$

The product  $\mathbf{a} \cdot \mathbf{a}^\dagger$  in (32.10) is equivalent to the following:  $\mathbf{a} \cdot \mathbf{a}^\dagger = \mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}$ ,

$$\text{therefore: } \mathbf{a}^\dagger \cdot \mathbf{a} \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle = \mathbf{a}^\dagger \cdot (\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}) | \varphi_\nu \rangle = \mathbf{a}^\dagger \cdot (\mathbf{I} + \mathbf{N}) | \varphi_\nu \rangle,$$

$$\text{from (32.10) the equality: } \mathbf{N} \cdot \mathbf{a}^\dagger = \mathbf{a}^\dagger \cdot (\mathbf{N} + \mathbf{I}). \text{ The eigenvalues equation gives:} \quad (32.11)$$

$$\mathbf{N} \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle = \mathbf{a}^\dagger \cdot (\mathbf{N} + \mathbf{I}) | \varphi_\nu \rangle = \mathbf{a}^\dagger \cdot (\nu + 1) | \varphi_\nu \rangle = (\nu + 1) \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle$$

$$\text{finally resulting: } \mathbf{N} \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle = (\nu + 1) \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle$$

so that  $\mathbf{a}^\dagger | \varphi_\nu \rangle$  is an eigenvector of  $\mathbf{N}$  with eigenvalue  $\nu + 1$ . In that case I can define the new eigenvectors

$$| \varphi_{\nu+1} \rangle = \mathbf{a}^\dagger | \varphi_\nu \rangle \quad (32.12)$$

$$| \varphi_{\nu+2} \rangle = (\mathbf{a}^\dagger)^2 | \varphi_\nu \rangle \quad (32.13)$$

$$| \varphi_{\nu+m} \rangle = (\mathbf{a}^\dagger)^m | \varphi_\nu \rangle \quad (32.14)$$

Resuming the previous results (32.9) and (32.14):

$$| \varphi_{\nu-m} \rangle = \mathbf{a}^m | \varphi_\nu \rangle \quad \text{eigenvalues } \nu-m \quad (32.9)$$

$$| \varphi_{\nu+m} \rangle = (\mathbf{a}^\dagger)^m | \varphi_\nu \rangle \quad \text{eigenvalues } \nu+m \quad (32.14)$$

$$| \varphi_{\nu+m} \rangle \neq | 0 \rangle \quad (32.15)$$

☑ Demonstration of  $|\varphi(\lambda+m)\rangle \neq |0\rangle$

$$\text{In fact assume } \mathbf{a}^\dagger | \varphi_\nu \rangle = | 0 \rangle, \text{ then } (\| \mathbf{a}^\dagger | \varphi_\nu \rangle \|^2) = (\langle \varphi_\nu | \mathbf{a} \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle)^2$$

$$\langle \varphi_\nu | \mathbf{a} \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle = \langle \varphi_\nu | (\mathbf{a} \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle)$$

$$\mathbf{a} \cdot \mathbf{a}^\dagger = \mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}$$

$$\langle \varphi_\nu | \mathbf{a} \cdot \mathbf{a}^\dagger | \varphi_\nu \rangle = \langle \varphi_\nu | [(\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}) | \varphi_\nu \rangle] = \langle \varphi_\nu | \mathbf{a}^\dagger \cdot \mathbf{a} | \varphi_\nu \rangle + \langle \varphi_\nu | \mathbf{I} | \varphi_\nu \rangle$$

$$\langle \varphi_\nu | \mathbf{a}^\dagger \cdot \mathbf{a} | \varphi_\nu \rangle + \langle \varphi_\nu | \mathbf{I} | \varphi_\nu \rangle = (\| \mathbf{a} | \varphi_\nu \rangle \|^2) + (\| | \varphi_\nu \rangle \|^2) \neq | 0 \rangle \quad \text{since } | \varphi_\nu \rangle \neq | 0 \rangle$$

☑ Demonstration of  $|\varphi(\lambda+m)\rangle \neq |0\rangle$

Finally, results  $| \varphi_{\nu+1} \rangle$  always an eigenvector of  $\mathbf{N}$  with eigenvalue  $\nu+1$ . On the other hand  $| \varphi_{\nu-m} \rangle$  can be zero. In fact, calculate the average:

$$\langle \varphi_{\nu-m} | \mathbf{N} | \varphi_{\nu-m} \rangle = \langle \varphi_{\nu-m} | (\nu - m) | \varphi_{\nu-m} \rangle = (\nu - m) \langle \varphi_{\nu-m} | \varphi_{\nu-m} \rangle \quad (32.16)$$

$$\text{this result can be rewritten as: } (\nu - m) \langle \varphi_{\nu-m} | \varphi_{\nu-m} \rangle = (\nu - m) \cdot (\| | \varphi_{\nu-m} \rangle \|^2) \quad (32.17)$$

$$\text{in such a way that: } \nu - m = \frac{\langle \varphi_{\nu-m} | \mathbf{N} | \varphi_{\nu-m} \rangle}{(\| | \varphi_{\nu-m} \rangle \|^2)} \quad (32.18)$$

On the other hand the average of the operator  $\mathbf{N}$  is:

$$\langle \varphi_{\nu-m} | \mathbf{N} | \varphi_{\nu-m} \rangle = \langle \varphi_{\nu-m} | \mathbf{a}^\dagger \cdot \mathbf{a} | \varphi_{\nu-m} \rangle = (\| \mathbf{a} | \varphi_{\nu-m} \rangle \|^2) \quad (32.19)$$

$$\text{so that I can write as well: } \nu - m = \frac{(\| \mathbf{a} | \varphi_{\nu-m} \rangle \|^2)}{(\| | \varphi_{\nu-m} \rangle \|^2)} \geq 0 \quad (32.20)$$

It follows that the sequence of eigenvectors  $| \varphi_{\nu-m} \rangle$ , must terminate after a finite number of steps and there must exist one vector  $| \varphi_0 \rangle$  such that  $\mathbf{a} | \varphi_0 \rangle = | 0 \rangle$ .

**Normalization:**

$$\text{define the normalized eigenvector as } | \phi_0 \rangle = \frac{| \varphi_0 \rangle}{\| | \varphi_0 \rangle \|} = C_0 | \phi_0 \rangle \quad C_0 = 1 \quad (32.21)$$

☑ Various cases

Since holds (3.14)  $(\mathbf{a}^\dagger)^m | \varphi_\nu \rangle = | \varphi_{\nu+m} \rangle$ , for  $\nu = 0$  and  $m = 1$ , I get:  $\mathbf{a}^\dagger | \varphi_0 \rangle = | \varphi_1 \rangle$ .

$$\text{Normalization: } | \phi_1 \rangle = \frac{| \varphi_1 \rangle}{\| | \varphi_1 \rangle \|} = \frac{\mathbf{a}^\dagger | \varphi_0 \rangle}{\| \mathbf{a}^\dagger | \varphi_0 \rangle \|} \quad (32.21')$$

Since  $\exists k_1 \in \mathbb{C}: \| \mathbf{a}^\dagger | \varphi_0 \rangle \| \leq |k_1| \| | \varphi_0 \rangle \|, \forall | \varphi_0 \rangle \in \mathbb{H}$ , assuming the equality, I can write:

$$\frac{\mathbf{a}^\dagger | \varphi_0 \rangle}{\| \mathbf{a}^\dagger | \varphi_0 \rangle \|} = \frac{\mathbf{a}^\dagger | \varphi_0 \rangle}{|k_1| \| | \varphi_0 \rangle \|} = C_1 \cdot \mathbf{a}^\dagger | \phi_0 \rangle$$

$$C_1 = \frac{1}{|k_1|}$$

For  $\nu = 0$  and  $m = 2$ , I get:  $(\mathbf{a}^\dagger)^2 | \varphi_0 \rangle = | \varphi_2 \rangle$ .

$$\text{Normalization: } | \phi_2 \rangle = \frac{| \varphi_2 \rangle}{\| | \varphi_2 \rangle \|} = \frac{(\mathbf{a}^\dagger)^2 | \varphi_0 \rangle}{\| (\mathbf{a}^\dagger)^2 | \varphi_0 \rangle \|} \quad (32.21'')$$

Since  $\exists k_2 \in \mathbb{C}: \| (\mathbf{a}^\dagger)^2 | \varphi_0 \rangle \| \leq |k_2| \| | \varphi_0 \rangle \|, \forall | \varphi_0 \rangle \in \mathbb{H}$ , assuming the equality, I can write:

$$\frac{(\mathbf{a}^\dagger)^2 | \varphi_0 \rangle}{\| (\mathbf{a}^\dagger)^2 | \varphi_0 \rangle \|} = \frac{(\mathbf{a}^\dagger)^2 | \varphi_0 \rangle}{k_2 \| | \varphi_0 \rangle \|} = C_2 \cdot (\mathbf{a}^\dagger)^2 | \phi_0 \rangle$$

$$C_2 = \frac{1}{k_2}$$

$$\text{Normalization: } |\phi_{n-1}\rangle = \frac{|\varphi_{n-1}\rangle}{\| |\varphi_{n-1}\rangle \|} = \frac{(\mathbf{a}^\dagger)^{n-1} |\varphi_0\rangle}{\| (\mathbf{a}^\dagger)^{n-1} |\varphi_0\rangle \|}$$

Since  $\exists k_{n-1} \in \mathbb{C}: \| (\mathbf{a}^\dagger)^{n-1} |\varphi_0\rangle \| \leq |k_{n-1}| \| |\varphi_0\rangle \|, \forall |\varphi_0\rangle \in \mathbb{H}$ , assuming the equality, I can write:

$$\frac{(\mathbf{a}^\dagger)^{n-1} |\varphi_0\rangle}{\| (\mathbf{a}^\dagger)^{n-1} |\varphi_0\rangle \|} = \frac{(\mathbf{a}^\dagger)^{n-1} |\varphi_0\rangle}{k_{n-1} \| |\varphi_0\rangle \|} = C_{n-1} \cdot (\mathbf{a}^\dagger)^{n-1} |\varphi_0\rangle$$

$$|\phi_{n-1}\rangle = C_{n-1} \cdot (\mathbf{a}^\dagger)^{n-1} |\varphi_0\rangle$$

$$C_{n-1} = \frac{1}{k_{n-1}}$$

Various cases

$$\text{generalizing I get: } |\phi_n\rangle = \frac{|\varphi_n\rangle}{\| |\varphi_n\rangle \|} = C_n \cdot (\mathbf{a}^\dagger)^n |\varphi_0\rangle \quad (32.22)$$

$$|\phi_n\rangle = C_n \cdot (\mathbf{a}^\dagger)^n |\varphi_0\rangle \quad (32.23)$$

$$C_n = \frac{1}{k_n}$$

I'm looking for a relation between  $C_n$  and  $C_{n-1}$ . Consider therefore the normalization of the eigenvalue equation with  $\nu = n$ :

$$\frac{N |\varphi_n\rangle}{\| |\varphi_n\rangle \|} = \frac{n |\varphi_n\rangle}{\| |\varphi_n\rangle \|} \quad (32.24)$$

thanks to (32.22) eq. (32.24) it can be rewritten:

$$N |\phi_n\rangle = n |\phi_n\rangle \quad (32.25)$$

$$\text{whose norm is: } \| |\phi_n\rangle \| = \sqrt{\langle \phi_n | \phi_n \rangle} = 1 \quad (32.26)$$

Now calculate the square of (32.26) and substitute in it eq.(32.23):

$$(\| |\phi_n\rangle \|^2) = \left[ \| C_n (\mathbf{a}^\dagger)^n |\varphi_0\rangle \|^2 \right] = (|C_n|)^2 \cdot \langle \phi_0 | (\mathbf{a} \cdot \mathbf{a}^\dagger)^n | \phi_0 \rangle = 1 \quad (32.27)$$

Calculation of  $\| |\phi\rangle \|^2$

$$\| C_n (\mathbf{a}^\dagger)^n | \phi_0 \rangle \|^2 = \left[ C_n (\mathbf{a}^\dagger)^n | \phi_0 \rangle \right]^\dagger C_n (\mathbf{a}^\dagger)^n | \phi_0 \rangle = \langle \phi_0 | (C_n^*) \cdot \left[ (\mathbf{a}^\dagger)^\dagger \right]^n \cdot C_n (\mathbf{a}^\dagger)^n | \phi_0 \rangle$$

$$\left[ (\mathbf{a}^\dagger)^\dagger \right]^n \cdot (\mathbf{a}^\dagger)^n = (\mathbf{a})^n \cdot (\mathbf{a}^\dagger)^n = (\mathbf{a} \cdot \mathbf{a}^\dagger)^n$$

$$\langle \phi_0 | (C_n^*) \cdot \left[ (\mathbf{a}^\dagger)^\dagger \right]^n \cdot C_n (\mathbf{a}^\dagger)^n | \phi_0 \rangle = \langle \phi_0 | (C_n^*) \cdot \mathbf{a}^n \cdot C_n (\mathbf{a}^\dagger)^n | \phi_0 \rangle$$

$$\langle \phi_0 | C_n^* \cdot \mathbf{a}^n \cdot C_n (\mathbf{a}^\dagger)^n | \phi_0 \rangle = C_n^* \cdot C_n \langle \phi_0 | (\mathbf{a} \cdot \mathbf{a}^\dagger)^n | \phi_0 \rangle = (|C_n|)^2 \langle \phi_0 | (\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a})^n | \phi_0 \rangle$$

Calculation of  $\| |\phi\rangle \|^2$

In the average (32.27) there is the previously defined ket (32.23):

$$(\mathbf{a}^\dagger)^n | \phi_0 \rangle = \frac{1}{C_n} | \phi_n \rangle = \frac{\mathbf{a}^\dagger | \phi_{n-1} \rangle}{C_{n-1}} \quad (32.28)$$

which substituted in the result (32.27), gives:

$$\langle \phi_0 | (\mathbf{a} \cdot \mathbf{a}^\dagger)^n | \phi_0 \rangle = \frac{1}{(|C_n|)^2} = \frac{\langle \phi_{n-1} | \mathbf{a} \cdot \mathbf{a}^\dagger | \phi_{n-1} \rangle}{(|C_{n-1}|)^2} = \frac{\langle \phi_{n-1} | (\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}) | \phi_{n-1} \rangle}{(|C_{n-1}|)^2}$$

$$(|C_n|)^2 \cdot \left[ \langle \phi_0 | (\mathbf{a} \cdot \mathbf{a}^\dagger)^n | \phi_0 \rangle \right]^2 = (|C_n|)^2 \cdot (\langle \phi_n | \phi_n \rangle)^2 = (|C_n|)^2 = 1$$

$$\frac{1}{(|C_n|)^2} = n \cdot \frac{\langle \phi_{n-1} | \phi_{n-1} \rangle}{(|C_{n-1}|)^2} = \frac{n}{(|C_{n-1}|)^2} \quad \langle \phi_{n-1} | \phi_{n-1} \rangle = 1$$

$$\frac{\langle \phi_{n-1} | (\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}) | \phi_{n-1} \rangle}{(|C_{n-1}|)^2} = \frac{\langle \phi_{n-1} | (N + 1) | \phi_{n-1} \rangle}{(|C_{n-1}|)^2} = n \cdot \frac{\langle \phi_{n-1} | \phi_{n-1} \rangle}{(|C_{n-1}|)^2}$$

<n|

$$\left[ (\mathbf{a}^\dagger)^n | \phi_0 \rangle \right]^\dagger = \langle \phi_0 | \left[ (\mathbf{a}^\dagger)^n \right]^\dagger = \langle \phi_0 | \mathbf{a}^n = \langle \phi_n |$$

<n|

Sequence

$$\begin{aligned} \frac{n \cdot (|C_n|)^2}{(|C_{n-1}|)^2} &= 1 & n \cdot (|C_n|)^2 &= (|C_{n-1}|)^2 \\ |C_n| &= \frac{1}{\sqrt{n}} \cdot |C_{n-1}| & |C_0| &= 1 \\ n=1 & & |C_1| &= |C_0| = 1 \\ n=2 & & |C_2| &= \frac{1}{\sqrt{2}} \\ n=3 & & |C_3| &= \frac{1}{\sqrt{3}} \cdot |C_2| = \frac{1}{\sqrt{3}} \cdot \frac{1}{\sqrt{2}} \\ n=4 & & |C_4| &= \frac{1}{\sqrt{4}} \cdot |C_3| = \frac{1}{\sqrt{4}} \cdot \frac{1}{\sqrt{3}} \cdot \frac{1}{\sqrt{2}} \end{aligned}$$

$$C_n = \frac{1}{\sqrt{n!}} \quad (32.29)$$

The sought eigenvector is:  $|\phi_n\rangle = \frac{1}{\sqrt{n!}} \cdot (\mathbf{a}^\dagger)^n |\phi_0\rangle$  with eigenvalue n, (32.30)

(that is the solution of the eigenvalues equation:  $\mathbf{N} |\phi_n\rangle = n |\phi_n\rangle$ .)

They are orthonormal  $\langle \phi_n | \phi_\nu \rangle = \delta_{n,\nu}$  and form an orthonormal basis in Hilbert space  $\mathbb{H}$ , the space of the dynamical states of the quantum system under study. The operators  $\mathbf{a}$  and  $\mathbf{a}^\dagger$  are defined on this basis.

$$C |\phi_{\nu-1}\rangle = \mathbf{a} |\phi_\nu\rangle$$

$$\langle \phi_{\nu-1} | C \cdot C | \phi_{\nu-1} \rangle = \langle \phi_\nu | \mathbf{a}^\dagger \cdot \mathbf{a} | \phi_\nu \rangle = \langle \phi_\nu | \mathbf{N} | \phi_\nu \rangle = n \langle \phi_\nu | \phi_\nu \rangle$$

$$(|C|)^2 \langle \phi_{\nu-1} | \phi_{\nu-1} \rangle = n \langle \phi_\nu | \phi_\nu \rangle \quad \langle \phi_{\nu-1} | \phi_{\nu-1} \rangle = 1 \quad \langle \phi_\nu | \phi_\nu \rangle = 1$$

$$C = \sqrt{n}$$

$$C_1 |\phi_{\nu-1}\rangle = \mathbf{a}^\dagger |\phi_\nu\rangle$$

$$\langle \phi_{\nu-1} | C_1 \cdot C_1 | \phi_{\nu-1} \rangle = \langle \phi_\nu | \mathbf{a} \cdot \mathbf{a}^\dagger | \phi_\nu \rangle$$

$$\mathbf{a} \cdot \mathbf{a}^\dagger = \mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}$$

$$\langle \phi_{\nu-1} | C_1 \cdot C_1 | \phi_{\nu-1} \rangle = \langle \phi_\nu | \mathbf{a} \cdot \mathbf{a}^\dagger | \phi_\nu \rangle = \langle \phi_\nu | (\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}) | \phi_\nu \rangle = n \langle \phi_\nu | \phi_\nu \rangle$$

$$(|C_1|)^2 \langle \phi_{\nu-1} | \phi_{\nu-1} \rangle = \langle \phi_\nu | (\mathbf{I} + \mathbf{N}) | \phi_\nu \rangle = (n+1) \langle \phi_\nu | \phi_\nu \rangle$$

$$|C_1| = \sqrt{n+1}$$

(Ladder operators)  $\mathbf{a} |\phi_n\rangle = \sqrt{n} |\phi_{n-1}\rangle$  annihilation operator (32.31)

$\mathbf{a}^\dagger |\phi_n\rangle = \sqrt{n+1} |\phi_{n+1}\rangle$  creation operator (32.32)

Consider the set of all vectors  $|\Psi\rangle = \sum_{n=0}^{\infty} (\alpha_n |\phi_n\rangle)$  where the  $\alpha_n$  are complex numbers and

$$\sum_{n=0}^{\infty} [(|\alpha_n|)^2] < \infty$$

It forms a linear space, that is the Hilbert space  $\mathbb{H}$  spanned by  $|\phi_n\rangle$

The space of all  $|\Psi\rangle$  for which

$$\sum_{n=0}^{\infty} [(|\alpha_n|)^2 \cdot (n+1)^p] < \infty \quad p = 0, 1, 2, 3, \dots, \infty$$

will be denoted by  $\Sigma$  (Schwartz space)  $\Sigma \subset \mathbb{H}$ .

All the operators representing observables can be defined on the whole space  $\Sigma$  but not on all  $\mathbb{H}$ .

All observables are functions of the operators  $\mathbf{a}$  and  $\mathbf{a}^\dagger$  given by (32.31) and (32.32) known for all  $|\Psi\rangle$ .

Calculation of the diagonal matrix elements:

$$\mathbf{H} = \hbar \cdot \omega \cdot \mathbf{H}_0 = \hbar \cdot \omega \cdot \left( \mathbf{N} + \frac{1}{2} \cdot \mathbf{I} \right) \quad \mathbf{N} |\varphi_\nu\rangle = \nu |\varphi_\nu\rangle$$

$$\mathbf{H} |\phi_n\rangle = \hbar \cdot \omega \cdot \left( \mathbf{N} + \frac{1}{2} \cdot \mathbf{I} \right) |\phi_n\rangle = \hbar \cdot \omega \cdot \left( \nu + \frac{1}{2} \right) |\phi_n\rangle$$

$$\langle \phi_\nu | \mathbf{H} | \phi_\nu \rangle = \hbar \cdot \omega \langle \phi_\nu | \left( \mathbf{N} + \frac{1}{2} \cdot \mathbf{I} \right) | \phi_\nu \rangle = \hbar \cdot \omega \cdot \left( \nu + \frac{1}{2} \right) \langle \phi_\nu | \phi_\nu \rangle = \hbar \cdot \omega \cdot \left( \nu + \frac{1}{2} \right) \cdot (|\varphi_\nu\rangle)^2$$

$$E_\nu = \langle \phi_\nu | \mathbf{H} | \phi_\nu \rangle = \hbar \cdot \omega \cdot \left( \nu + \frac{1}{2} \right) \quad (|\varphi_\nu\rangle)^2 = 1 \quad (32.33)$$

$$E_\nu = \Delta E \cdot \left( \nu + \frac{1}{2} \right) \quad \Delta E = \hbar \cdot \omega$$

the diagonal matrix elements are the possible energy values of the QM oscillator. One can excite the harmonic oscillator into any one of a discrete number of *states* described by  $|\phi_\nu\rangle$ , the system is in a mixture of states. The mixture can be described by the set of vectors  $|\phi_0\rangle, |\phi_1\rangle, |\phi_2\rangle, \dots, |\phi_\nu\rangle$  and a set of relative probabilities  $w_0, w_1, w_2, \dots, w_\nu, \dots$  proportional to the height of the jump corresponding to the energy  $E_n$ .

$$\sum_n w_n = 1$$

In a collection of N elements (atoms, molecules,) the number of elements with energy  $E_n$  is  $N_n = w_n N$ .

If no excitation take place, the harmonic oscillator is in the ground state described by  $|\phi_0\rangle$ , (See Frank

& Hertz experiment). If there is only one state  $|\phi_{n0}\rangle$  then the quantum system is in a *pure state*  $|\phi_{n0}\rangle$  and the corresponding energy is the only one  $E_{n0}$ .

**II axiom.** A physical QM system characterized by a projection operator  $\mathbf{P}$  on a one-dimensional subspace  $\mathbf{P}\mathbb{H}$  is in a pure state.



### 33 Algebra of the two-dimensional harmonic oscillator [7]



**Books**

- [1] Siegfried Flügge - *Matematische Methoden der Physik - I Analysis*. Springer - Verlag.
- [2] Bronstein - Smendjajew - *Taschenbuch der Mathematik* - Verlag Harry Deutsch.
- [3] Siegfried Flügge - *Practical Quantum Mechanics* - Springer - Verlag
- [4] Albert Messiah - *Quantum Mechanics* - Vol. I North - Holland Publishing company
- [5] Albert Messiah - *Quantum Mechanics* - Vol. II North - Holland Publishing company
- [6] Kenneth R. Lang - *Astrophysical Formulae* - Second ed. Springer - Verlag
- [7] Arno Bhöm - *Quantum Mechanics* - Springer - Verlag
- [8] Gianfranco Pradisi - *Lezioni di metodi matematici della fisica* - Edizioni Della Normale
- [9] Fritz Reinhardt, Heinrich Soeder - *Atlante di Matematica* - Editore Ulrico Hoepli Milano
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- [11] G. D. Coughlan, et alii-*The ideas of Particle Physics An introduction for Scientists*- Cambridge