Reference:C:\Users\Franc\new folder\unit vectors.xmcd
Reference:C:\Users\Franc\new folder\Periodic Table.xmcd

Equation Format

QUANTUM MECHANICS

GENERAL FORMALISM FORMULAE

PART ONE

Edited by F. M.

Remark:

*1: Vectors depending from time and position, 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 imeans Instead the arithmetic mean, that is

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

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

if $\boxed{z = a + j \cdot b}$ *then* $\boxed{z^* = a - j \cdot b}$ *while in "MAthcad" as* $\bar{z} = a - j \cdot b$.

Banach-Hilbert spaces

$\mathbb{N}$ 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

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

a^* indicates the complex conjugated of a

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

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

Cauchy convergence criterion for real sequences.

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

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

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

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 there is also defined the scalar product and consequently the norm, it ***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

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

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

and the operation of product between a vector and a scalar

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

$(\lambda, v) \longrightarrow \lambda v$

Banach-Hilbert spaces

Tensors

1 Vector spaces

The physical state of an object (for example the orientation of the spin of an atom) is represented by a state's vector in 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 $| x >$ (ket) while the linear vector space with $(L = \{ | x > \}) \in \mathbb{H}$. Any linear function f($| \psi >$) of the ket $| \psi >$, possesses the superposition property, namely

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

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 $f(| x >)$ defines the new vector (bra) $< f |$. The value taken by this function for ket $| \psi >$ is the number $< f | \psi >$.

To the dual space of L belongs the vector bra $< x |$, dual of the ket $| x >$. 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 indicated as a conjugation, namely the bra conjugate to the ket $| x >$ is represented by $< x |$. The correspondence is a linear, that is to the linear combination $\lambda_2 | x > + \lambda_2 | y > = | z >$ corresponds the bra conjugate

$$< z | = \lambda_2 * < x | + \lambda_2 * < y |.$$

To the ket $| 0 >$ corresponds the bra $< 0 |$ and vice versa. For the linearity, are necessary two operations: the sum $| x > + | y > = | z >$ and the product between a complex constant $\boldsymbol{\alpha} \in \mathbb{C}$, and the ket $| x >$, namely

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

Ket vectors properties

∃ Opposite	$-| x > +	x > =	0 >$	(1.2)
∃ Neutral element (sum)	$| 0 >$ namely $| 0 > + | x > = | x >$	(1.3)
Commutative (sum)	$| x > + | y > = | y > + | x >$	(1.4)
Associative (sum)	$(| x > + | y >) +	z > =	x > + (| y > + | z >)$	(1.5)
Distributive (sum)	$\alpha \cdot (| x > + | y >) = \alpha | x > + \alpha | y >$	(1.6)
Distributive (product)	$(\alpha + \beta) \cdot (| x >) = \alpha | x > + \beta | x >$	(1.7)
Associative (product)	$\alpha \cdot [\beta \cdot (| x >)] = (\alpha \cdot \beta) | x >$	(1.8)
	$1 \cdot (| x >) = | x >$	(1.9)

To the ket $| w > = \int_{\xi_1}^{\xi_2} \lambda(\xi) \cdot (| \xi >) \, d\xi$ corresponds the bra conjugated $< w | = \int_{\xi_1}^{\xi_2} \lambda(\xi) * \cdot (< \xi |) \, d\xi$

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

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

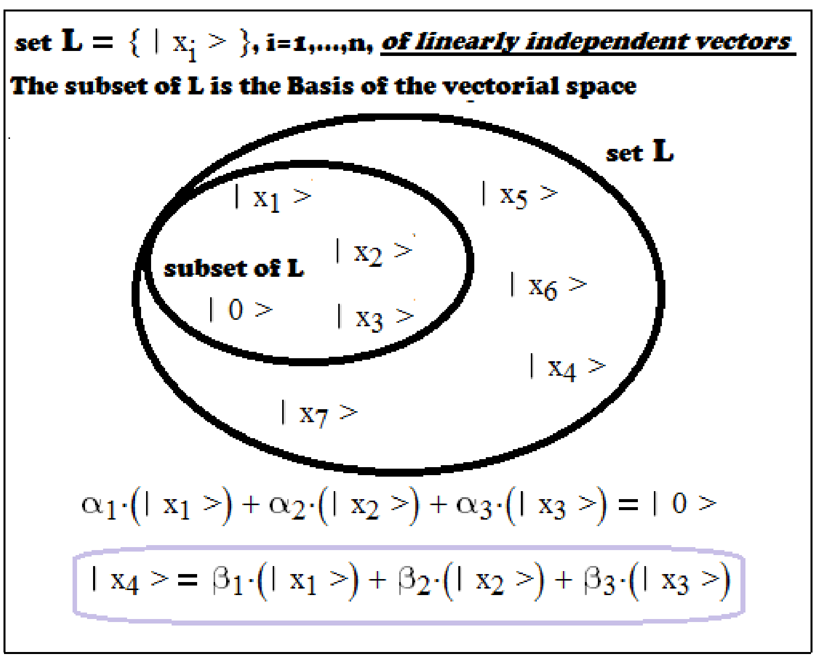
b) two and three-dimensional geometric spaces (•,+,-,/),

c) the set Mat of the square matrices (N x N) (•,+,-,inverse),
d) the set of all continuous functions defined on a continuous and established range (•,+,-,
e) the set of all integrable functions (•,+,-,/),
f) the set of all square integrable functions (•,+,-,/),
g) the set of all function families of functions (•,+,-,/).

Introducing in a set one or more composition laws (internal, external as addition and multiplication (•,+,-) of vectors b scalars for $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{R}$, $\mathbb{C}$), I give to the set an algebraic structure (The most important algebraic structures are: *group, semigroup, ring body, modulus, vector space*). More simply, an *Algebra* is created when I define the product among the elements of the set L and as result it gives a new element of the same set. It is an *external product* and not a scalar product (internal) [8].
A measure of the vectors is given by the scalar product.

A set $L = \{ | x_i > \}$, i=1,...,n, is *linearly independent* if and only if $\sum_{j=1}^{n} \left[\alpha_j \cdot (| x_j >)\right] = | 0 >$ which means that all the coefficients α_j are zero. The set L can also be infinite, but the sum must be carried on a finite set or subset of L than the set is linearly independent.
Definition of *Basis of a vector space* for finite or infinite dimensional spaces:
each set of linearly independent vectors such that any other vector of the space can be expressed as a linear combination of such vectors, is a base of a finite dimensional vector space.
Example of bases of finite dimensional vector spaces:

a_1) Geometrical spaces: each set of three non-coplanar vectors , constitutes a basis.
a_2) N-tuples (a collection of n ordered objects) of complex numbers $\alpha \in \mathbb{C}$, the base is a linear combination of the n-tuple.
a_3) Square matrix (N x N).
a_4) Polynomials (linear combinations of monomials) they have no finite dimension.
a_5) The space of the square summable functions hasn't finite dimension.



Let H_1 and H_2 be two vector spaces and the ket $| u > \in H_1$ and $| v > \in H_2$. Define the tensor product of the vecto spaces H_1 and H_2 as:

$$H_{12} = H_1 \otimes H_2$$

and the kets product (or tensor product) as:

$$| u v > = | u > | v >,$$

this product is commutative that is:

$$| \, u \, v > = | \, v \, u > \text{or} \; | \, u > | \, v > = | \, v > | \, u >,$$

it is distributive with respect to the sum:

$$| \, u > = \lambda | \, \xi > + \mu | \, \psi >,$$

$$| \, u \, v > = \left(\lambda | \, \xi > + \mu | \, \psi > \right) | \, v > = \lambda | \, \xi > | \, v > + \mu | \, \psi > | \, v >,$$

$$\text{while if} \quad | \, v > = \lambda | \, \xi > + \mu | \, \psi > \;,$$

$$| \, u \, v > = | \, u > \left(\lambda | \, \xi > + \mu | \, \psi > \right) = \lambda | \, u > | \, \xi > + \mu | \, u > | \, \psi >,$$

2 *Scalar product axioms* [4]

Scalar product (or internal product) of two vectors ($| x >, | y >$) belonging to the Euclidean and vector space $L = \{ | x > \}$. The scalar product must associate to each couple of vectors ($| x >, | y >$) a complex number, namely:

$$(| x >, | y >) \to \alpha = < x | y >$$

$$< x | y > = < x | \cdot (| y >) \tag{2.1}$$

$$< x | x > \geq 0 \tag{2.2}$$

$$< x | x > = 0 \quad \Rightarrow \quad | x > = | 0 > \tag{2.3}$$

$$< x | y > = < y | x > * \tag{2.4}$$

$$< x | (\alpha \cdot y) > = \alpha \cdot (< x | y >) \tag{2.5}$$

$$< (\alpha \cdot x) | y > = \alpha * \cdot (< x | y >) \tag{2.6}$$

$$< x | (y + z) > = < x | y > + < x | z > \tag{2.7}$$

Norm $$\| \, | x > \| = \sqrt{< x | x >} \qquad 0 \leq \| \, | x > \| \leq \infty \tag{2.8}$$

$$\| \, \alpha \cdot (| x >) \, \| = |\alpha| \cdot (\| \, | x > \|) \tag{2.9}$$

Triangular inequality $$\| \, | x > + | y > \| \leq \| \, | x > \| + \| \, | y > \| \tag{2.10}$$

Distance $$d_{xy} = \| \, | x > - | y > \| \tag{2.11}$$

External product between a ket $| x >$ and a bra $< x |$ is the operator: $| x > < x |$. (2.12)

3 *vector analysis*

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

$$\lim_{n \to \infty} | x_n > = | x > \Leftrightarrow \lim_{n \to \infty} \| \, | x_n > - | x > \| = 0. \tag{3.1}$$

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

$$\lim_{t \to t_0} | x(t) > = | x > \tag{3.2}$$

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 $| x(t) > = | t >$, $| x_1 > = | 1 >$,... So, I can write:

$$\lim_{t \to t_0} | t > = | t_0 >, \ \forall \varepsilon > 0, \exists \delta_\varepsilon > 0 : \ |t - t_0| < \delta \Rightarrow \left| | t > - | t_0 > \right| < \varepsilon. \tag{3.3}$$

Derivative

$$\frac{d}{dt} | t > = \lim_{t \to t_0} \frac{| t > - | t_0 >}{t - t_0}, \text{ etc.} \tag{3.4}$$

Integral in (a,b):

consider the function $\sum_{k=1}^{n} \left[\left(t_k - t_{k-1} \right) \mid t_k > \right]$, $t_0 = a$, $t_n = b$, (3.5)

if exists the limit $$\lim_{\left|\delta_k\right| \to 0} \sum_{k=1}^{n} \left[\left(t_k - t_{k-1} \right) \mid t_k > \right] = \int \mid t > dt = \mid Q > \qquad (3.6)$$

then $\mid Q >$ is the integral of $\mid t >$.

In (a,b): $$\mid Q(b) > - \mid Q(a) > = \int_a^b \mid t > dt. \qquad (3.7)$$

Derivative and integral are linear operators.

4 Orthogonal systems of vectors

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

$$\forall \alpha, \beta \in \left(\mathbb{R}^2\right), < x_\alpha | x_\beta > = \delta_{\alpha\beta} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ for } \begin{pmatrix} \alpha \neq \beta \\ \alpha = \beta \end{pmatrix}. \tag{4.1}$$

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.

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

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

$$< a | b > = \sum_{n=1}^{\infty} \left(a_n * \cdot b_n\right), \tag{4.2}$$

$$< a | (\alpha \cdot b) > = \sum_{n=1}^{\infty} \left(a_n * \cdot \alpha \cdot b_n\right) = \alpha \cdot \sum_{n=1}^{\infty} \left(a_n * \cdot b_n\right), \tag{4.3}$$

$$< (\alpha \cdot a) | b > = \sum_{n=1}^{\infty} \left[\left(\alpha \cdot a_n\right) * \cdot b_n\right] = \alpha * \cdot \sum_{n=1}^{\infty} \left(a_n * \cdot b_n\right), \tag{4.4}$$

$$\text{Cauchy criterion: } \forall \varepsilon > 0, \exists N \geq 1 (\in) \mathbb{Z} : \left|a_n - a\right| \leq \varepsilon, \forall n \geq N \Rightarrow \lim_{n \to \infty} a_n = a. \tag{4.5}$$

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

$$\forall \varepsilon > 0, \exists N \geq 1 (\in) \mathbb{Z} : \left|b_n - b\right| \leq \varepsilon, \forall n \geq N \Rightarrow \lim_{n \to \infty} b_n = b.$$

$$\forall \varepsilon > 0, \exists N \geq 1 (\in) \mathbb{Z} : \left|b_n - b_m\right| \leq \varepsilon, \forall n, m \geq N \Rightarrow \lim_{n \to \infty} b_n = b.$$

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

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

$$\boxed{< f | g > = \int_0^1 f(x) * \cdot g(x)\, dx}\ , \tag{4.6}$$

which always exists, been f and g continue functions.

Now see if they satisfy the scalar product axioms:

$$< f | (\alpha \cdot g) > = \int_0^1 f(x) * \cdot \alpha \cdot g(x)\, dx = \alpha \cdot \int_0^1 f(x) * \cdot g(x)\, dx = \alpha \cdot \left(< f(x) | g(x) >\right), \tag{4.7}$$

$$< (\alpha \cdot f) | g > = \int_0^1 (\alpha \cdot f(x)) * \cdot g(x)\, dx = \alpha * \cdot \int_0^1 f(x) * \cdot g(x)\, dx = \alpha * \cdot \left(< f(x) | g(x) >\right), \tag{4.8}$$

$$< f | f > \geq 0, \tag{4.9}$$

and so on.

If the Cauchy's convergence criterion is verified, then this vector space is complete and, therefore the continue functions' space is a Hilbert space.

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

$L^2[\,0,2\cdot\pi\,] \supset \{ \dfrac{e^{i\cdot n\cdot x}}{\sqrt{2\cdot\pi}} \}$ is a complete space 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.

$$P(n,x) = \frac{1}{2^n\cdot n!}\cdot\frac{\partial^n}{\partial x^n}\left(x^2-1\right)^n,\ \ f(n,x) = \sqrt{n+\frac{1}{2}}\cdot P(n,x). \tag{4.10}$$

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

$$H(n,z) = \frac{e^{z^2}}{\sqrt{2^n\cdot n!\cdot\pi}}\cdot\frac{\partial^n}{\partial z^n}e^{-z^2} = (-1)^n\cdot\frac{2\cdot n!}{n!}\cdot F\left(-n,\frac{1}{2},z^2\right). \tag{4.11}$$

5 *Limited linear operators* [8]

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

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

The eigenvalues spectrum consists of:

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

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

Properties of the continuous spectrum:

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

2) orthonormality of the eigenkets belonging to distinct eigenvalues: $< y(\nu, r) \mid y(\nu_1, r_1) > = \Delta(\nu, \nu_1)\cdot\Delta(r, r_1)$

A linear application $\mathbf{A} : \mathbb{H}_1 \rightarrow \mathbb{H}_2$ (**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.

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

The set of all limited and linear operators, together the usual composition laws, is indicated with $[H_1,H_2]$.

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

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

$$\forall \mid x > \in D_A \subset \mathbb{H}_1 \Rightarrow \mathbf{A} \mid x > \in \mathfrak{R}(\mathbf{A}) \subset \mathbb{H}_2.$$

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

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

$$(\mathbf{A}\cdot\mathbf{B}) \mid x > = \mathbf{A}\cdot(\mathbf{B} \mid x >), \quad (5.4)$$

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

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

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

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

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

Identity $\mathbf{A}\cdot\mathbf{I} = \mathbf{A}$, (5.10)

Example matrix calculation

Schwarz inequality [4] $(|< x \mid \mathbf{A} \mid y >|)^2 \leq < x \mid \mathbf{A} \mid x > \bullet (< y \mid \mathbf{A} \mid y >)$ (5.11)

Bessel inequality [4] $\sum_\alpha \left[(|< x_\alpha \mid x >|)^2\right] \leq < x \mid x > \quad \forall \mid x > \ (\forall \mid x_\alpha > \neq 0)\ (\in)\ L$ (5.12)

Parseval Theorem [4] $\sum_\alpha (|< x_\alpha \mid x >|)^2 = < x \mid x >$ (5.13)

then the orthonormal system is complete. In such case is worth the following vector decomposition:

Decomposition $\mid x > = \sum_\alpha < x_\alpha \mid x > \mid x_\alpha > \quad \forall \mid x > \ (\forall \mid x_\alpha > \neq 0)\ (\in)\ L$ (5.14)

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

$$(L = \{ \mid x(t) > \}) \in \mathbb{H},$$

is a complete basis.

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

$$\forall\,|\,x>,\quad \forall\,|\,x_j>\neq 0\in L=\{\,|\,x(t)>\}\in\mathbb{H}\Rightarrow\,|\,x>=\sum_{j=0}^{N}<x_j\,|\,x>|\,x_j>. \tag{5.15}$$

$$|\,x>=|\,x_s>+|\,x_n> \tag{5.16}$$

$$\left(<x_s\,|\,x_s>\right)^2+\left(<x_n\,|\,x_n>\right)^2\leq\left(\left|<x\,|\,x>\right|\right)^2$$

$$<x_s\,|\,x_n>=0 \tag{5.17}$$

6 Inverse operators

Inverse operator $\mathbf{A}^{-1}$, is an operator such that $\mathbf{A}^{-1}\cdot\mathbf{A}=\mathbf{A}\cdot\mathbf{A}^{-1}=\mathbf{I}$, (6.1)
this property is not always verified (not invertible operator). That is the operator $\mathbf{A}$ is invertible if and only if

$$\forall\,|\,y>\in\left[\Re\,(\mathbf{A})\right]\exists\,|\,x>\in D_A\Rightarrow\mathbf{A}\,|\,x>=|\,y>\in\Re\,(\mathbf{A})\subset\mathbb{H}_2.$$

$$\mathbf{A}\,|\,x>=|\,y>\quad\Rightarrow\quad\left(\mathbf{A}^{-1}\cdot\mathbf{A}\right)|\,x>=|\,x>=\mathbf{A}^{-1}\,|\,y>.$$

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

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

$$(\mathbf{A}-\mathbf{B})^{-1}=\mathbf{A}^{-1}+\mathbf{A}^{-1}\cdot\mathbf{B}\cdot(\mathbf{A}-\mathbf{B})^{-1}. \tag{6.2}$$

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

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

$$\boxed{(\mathbf{A}-\mathbf{B})^{-1}=\left(\mathbf{I}-\mathbf{A}^{-1}\cdot\mathbf{B}\right)^{-1}\cdot\mathbf{A}^{-1}}$$

$$\boxed{(\mathbf{A}+\mathbf{B})^{-1}=\left(\mathbf{I}+\mathbf{A}^{-1}\cdot\mathbf{B}\right)^{-1}\cdot\mathbf{A}^{-1}}$$

$$\left(\mathbf{A}^2-\mathbf{B}^2\right)^{-1}=\left[(\mathbf{A}+\mathbf{B})\cdot(\mathbf{A}-\mathbf{B})+[\,\mathbf{A},\mathbf{B}\,]\right]^{-1}$$

$$\left(\mathbf{A}^2+\mathbf{B}^2\right)^{-1}=\left[(\mathbf{A}+i\cdot\mathbf{B})\cdot(\mathbf{A}-i\cdot\mathbf{B})+i\cdot\left([\,\mathbf{A},\mathbf{B}\,]\right)\right]^{-1}$$

The operator $\mathbf{P}=|\,u><v\,|$ has no inverse.

Examples of operators inversion:

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

Fourier $\mathfrak{F}=\int_{-\infty}^{\infty}e^{-i\cdot\omega\cdot x}\,dx$ use with the Mathcad prefix operator

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

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

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

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

Differential operators
Examples:

$Do_1)$

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

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

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

$D_A \in \mathbb{R}$ $\qquad Do_2)$

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

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

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

Example with matrices

7 Adjoint operator [4]

The **adjoint** of a linear operator **A** (or Hermitian conjugate operator of **A**) is written $\mathbf{A}^{\dagger}$ (read: adjoint of **A**).

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

furthermore, the operator A is ***Hermitian*** if $\qquad A = \mathbf{A}^{\dagger}.$

Let **A** be a linear operator and $|\,x>$ the ket conjugated of the bra $(<y\,|\,\mathbf{A})$, namely $|\,x> = (<y\,|\,\mathbf{A})^*$.
The ket $|\,x>$ depends anti linearly upon the bra $<y\,|$, it is therefore, a linear function of $|\,y>$, through the new operator $\mathbf{A}^{\dagger}$:

$$|\,x> = \mathbf{A}^{\dagger}\,|\,y> \qquad (7.2)$$

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

$$<u\,|\,\mathbf{A}\,|\,v> = <v\,|\,\mathbf{A}^{\dagger}\,|\,u> = <v\,|\,\mathbf{A}\,|\,u>^*. \qquad (7.3)$$

The ket conjugated to $<v\,|\,\mathbf{A}^{\dagger}$ is $\mathbf{A}\,|\,v>$.

practical rule to obtain the adjoint (or Hermitian conjugate)

of a const	replace with	const *complex conjugated

of a $< x \mid$ replace with $\mid x >$

of a $\mid x >$ replace with $< x \mid$

of a $\mathbf{A}$ 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

$$(\mathbf{A} \mid x >)^{\dagger} = < x \mid \mathbf{A}^{\dagger} \tag{7.5}$$

$$(< u \mid \mathbf{A} \mid v >)^{\dagger} = < v \mid \mathbf{A}^{\dagger} \mid u > \tag{7.6}$$

$$(\mathbf{A} \cdot \mathbf{B} \mid u >< v \mid \mathbf{C})^{\dagger} = \mathbf{C}^{\dagger} \mid v >< u \mid \mathbf{B}^{\dagger} \cdot \mathbf{A}^{\dagger} \tag{7.7}$$

$$(\mathbf{A} \cdot \mathbf{B} \mid u >< v \mid w >)^{\dagger} = < w \mid v >< u \mid \mathbf{B}^{\dagger} \cdot \mathbf{A}^{\dagger} \tag{7.8}$$

$$(< x \mid \mathbf{A} \cdot \mathbf{B} \mid u >< v \mid w >)^{\dagger} = < w \mid v >< u \mid \mathbf{B}^{\dagger} \cdot \mathbf{A}^{\dagger} \mid x > \tag{7.9}$$

$$(< x \mid \mathbf{A} \cdot \mathbf{B} \mid u >< v \mid \mathbf{C} \mid w >)^* = < w \mid \mathbf{C}^{\dagger} \mid v >< u \mid \mathbf{B}^{\dagger} \cdot \mathbf{A}^{\dagger} \mid x > \tag{7.10}$$

$$(< x \mid \mathbf{A} \cdot \mathbf{B} \mid u >< v \mid \mathbf{C} \mid w >)^* = < x \mid \mathbf{A} \cdot \mathbf{B} (\mid u >)^* \cdot < v \mid \mathbf{C} \mid w >^* \tag{7.11}$$

$$(< x \mid \mathbf{A} \cdot \mathbf{B} \mid u >)^{\dagger} = < u \mid \mathbf{B}^{\dagger} \cdot \mathbf{A}^{\dagger} \mid x > \tag{7.12}$$

$$(< v \mid \mathbf{C} \mid w >)^{\dagger} = < w \mid \mathbf{C}^{\dagger} \mid v > \tag{7.13}$$

$$< u \mid \mathbf{A} \mid v >^* = (< u \mid \mathbf{A} \mid v >)^{\dagger} = < v \mid \mathbf{A}^{\dagger} \mid u >$$

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 $< u \mid$ and $\mid v >$, as follows:

For $L^2 [\, a, b \,]$ the scalar product is
$$\boxed{< u \mid v > = \int_a^b u(x)^* \cdot v(x) \, dx} \tag{7.14}$$

according to the definition $< u \mid \mathbf{A} \mid v > = \int_a^b u(x)^* \cdot \mathbf{A} \, v(x) \, dx$ I proceed to calculate the adjoint:

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

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

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

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

$$< v \mid \mathbf{A}^\dagger \mid u > = \left(\int_a^b u(x)^*\cdot\mathbf{A}\,v(x)\,dx\right)^*$$

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

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,

$$\mathbf{A}^\dagger = c^*\cdot\mathbf{R}^\dagger \tag{7.17}$$

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

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

$$< v \mid \mathbf{A}^\dagger \mid u > = \left(c\cdot\int u^*\cdot\mathbf{R}\,v\,dx\right)^* = c^*\cdot\left[\left(u^*\cdot\int \mathbf{R}\,v\,dx\right)^* - \left[\int \left(\int \mathbf{R}\,v\,dx\right) du^*\right]^*\right]$$

$\mathbf{A} \in \left(L^2[\,a,b\,]\right)$

$$< v \mid \mathbf{A}^\dagger \mid u > = c^*\cdot\left[\lim_{x\to b}\left(u^*\cdot\int \mathbf{R}\,v\,dx\right)^* - \lim_{x\to a}\left(u^*\cdot\int \mathbf{R}\,v\,dx\right)^* - \left[\int_a^b \left(\int \mathbf{R}\,v\,dx\right) du^*\right]^*\right]$$

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

$$< u \mid \mathbf{A} \mid v >^* = \left(< u \mid \mathbf{A} \mid v >\right)^\dagger = < v \mid \mathbf{A}^\dagger \mid u > = \left[\int_a^b u(x)^*\cdot(\mathbf{Q}\cdot\mathbf{R})\,v(x)\,dx\right]^* \quad (\mathbf{Q},\mathbf{R}) \in \left(L^2[\,a,b\,]\right)$$

$$\left(< u \mid \mathbf{A} \mid v >\right)^\dagger = < v \mid (\mathbf{Q}\cdot\mathbf{R})^\dagger \mid u > = < v \mid \left(\mathbf{R}^\dagger\cdot\mathbf{Q}^\dagger\right) \mid u >$$

$$< v \mid \left(\mathbf{R}^\dagger\cdot\mathbf{Q}^\dagger\right) \mid u > = \int v^*\cdot\mathbf{R}^\dagger\cdot\mathbf{Q}^\dagger\,u\,dx = v^*\cdot\int \mathbf{R}^\dagger\cdot\mathbf{Q}^\dagger\,u\,dx - \int \left(\int \mathbf{R}^\dagger\cdot\mathbf{Q}^\dagger\,u\,dx\right) dv^*$$

calculate $\left(< u \mid \mathbf{A} \mid v >\right)^\dagger$ assuming that $(u,v) \in \left(L^2[\,a,b\,]\right)$ $\forall x \in ([\,a,b\,])$ $u(a) = u(b) = 0$

$$< v \mid \left(\mathbf{R}^{\dagger}\cdot\mathbf{Q}^{\dagger}\right) \mid u > = \lim_{x\to b}\left(v^{*}\cdot\int \mathbf{R}^{\dagger}\cdot\mathbf{Q}^{\dagger}\,u\,dx\right) - \lim_{x\to a}\left(v^{*}\cdot\int \mathbf{R}^{\dagger}\cdot\mathbf{Q}^{\dagger}\,u\,dx\right) \ldots$$

$$+\int_{a}^{b}\left(-\int \mathbf{R}^{\dagger}\cdot\mathbf{Q}^{\dagger}\,u\,dx\right)dv^{*}$$

3) $\mathbf{A} = F(x)\cdot\mathbf{R}$, $\mathbf{R}$ be the given vector Operator,

calculate $\left(< u \mid \mathbf{A} \mid v >\right)^{\dagger}$ assuming that $\left(F(x), u, v\right) \in \left(L^{2}[\,a, b\,]\right)$ $\forall x \in \left([\,a, b\,]\right)$ $u(a) = u(b) = 0$

$$\left(< u \mid \mathbf{A} \mid v >\right)^{\dagger} = < v \mid \mathbf{A}^{\dagger} \mid u > \qquad \mathbf{A}^{\dagger} = \left(F\cdot\mathbf{R}\right)^{\dagger} = F^{*}\cdot\mathbf{R}^{\dagger}$$

$$< v \mid \left(F^{*}\cdot\mathbf{R}^{\dagger}\right) \mid u > = \int v^{*}\cdot F^{*}\cdot\mathbf{R}^{\dagger}\,u\,dx = v^{*}\cdot\int F^{*}\cdot\mathbf{R}^{\dagger}\,u\,dx - \int\left(\int F^{*}\cdot\mathbf{R}^{\dagger}\,u\,dx\right)dv^{*}$$

$$< v \mid \left(F^{*}\cdot\mathbf{R}^{\dagger}\right) \mid u > = \lim_{x\to b}\left(v^{*}\cdot\int F^{*}\cdot\mathbf{R}^{\dagger}\,u\,dx\right) - \lim_{x\to a}\left(v^{*}\cdot\int F^{*}\cdot\mathbf{R}^{\dagger}\,u\,dx\right) \ldots$$

$$+\int_{a}^{b}\left(-v^{*}\cdot\int F^{*}\cdot\mathbf{R}^{\dagger}\,u\,dx\right)dv^{*}$$

4) $\mathbf{A} = \mathbf{Q} + \mathbf{R}$, $\mathbf{A} \in \left(L^{2}[\,a, b\,]\right)$ $\mathbf{Q}, \mathbf{R}$ be two vector Operators

$$< v \mid \left(\mathbf{Q}^{\dagger} + \mathbf{R}^{\dagger}\right) \mid u > = \int v^{*}\cdot\left(\mathbf{Q}^{\dagger} + \mathbf{R}^{\dagger}\right)u\,dx = v^{*}\cdot\int \left(\mathbf{Q}^{\dagger} + \mathbf{R}^{\dagger}\right)u\,dx - \int\left[\int \left(\mathbf{Q}^{\dagger} + \mathbf{R}^{\dagger}\right)v\,dx\right]dv^{*}$$

$\mathbf{A} \in \left(L^{2}[\,a, b\,]\right)$

$$< v \mid \left(\mathbf{Q}^{\dagger} + \mathbf{R}^{\dagger}\right) \mid u > = \lim_{x\to b}\left[v^{*}\cdot\int \left(\mathbf{Q}^{\dagger} + \mathbf{R}^{\dagger}\right)u\,dx\right] \ldots$$

$$+(-1)\cdot\lim_{x\to a}\left[v^{*}\cdot\int \left(\mathbf{Q}^{\dagger} + \mathbf{R}^{\dagger}\right)u\,dx\right] - \int_{a}^{b}\left[v^{*}\cdot\int \left(\mathbf{Q}^{\dagger} + \mathbf{R}^{\dagger}\right)u\,dx\right]du^{*}$$

8 Examples of adjoint operators calculation

Examples of adjoint operators calculation

Example Adj$_1$) [7]

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

calculate $< u \mid \mathbf{A}^\dagger \mid v >$ assuming that $(u, v) \in (L^2 [\, a, b\,])$ $\forall x \in ([\, a, b\,])$ $u(a) = u(b) = 0$

according to the definition: $< v \mid \mathbf{A}^\dagger \mid u > = \left[< u \mid (-i)\cdot\frac{\partial}{\partial x} \mid v >\right] * = \left(i\cdot\int_a^b u(x) * \frac{\partial}{\partial x} v(x)\, dx\right) *$

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

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

$$< v \mid \mathbf{A}^\dagger \mid u > = -i\cdot\left[\lim_{x \to b}\left(u * *\cdot\int \frac{\partial}{\partial x} v\, dx *\right) - \lim_{x \to a}\left(u * *\cdot\int \frac{\partial}{\partial x} v\, dx *\right)\right] \ldots$$
$$+ \left[\int_a^b \left(-\int \frac{\partial}{\partial x} v\, dx\right) du *\right] *$$

$$< v \mid \mathbf{A}^\dagger \mid u > = -i\cdot\left[\lim_{x \to b} (u\cdot v *) - \lim_{x \to a} (u\cdot v *) - \left[\int_a^b \left(\int \frac{\partial}{\partial x} v\, dx\right) du *\right] *\right]$$

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

$$< v \mid \mathbf{A}^\dagger \mid u > = i\cdot(v(b) *\cdot u(b) - v(a) *\cdot u(a)) - < u \mid i\cdot\frac{\partial}{\partial x} \mid v >$$

$$< v \mid \mathbf{A}^\dagger \mid u > = < u \mid i\cdot\frac{\partial}{\partial x} \mid v >$$

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

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

Example Adj$_2$) [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 $\boxed{P(x) \neq 0}$ $\boxed{Q(x) \neq 0}$ $\boxed{R(x) \neq 0}$

calculate $< u \mid \mathbf{A_x}^{\dagger} \mid v >$ assuming that $(u, v) \in \left(L^2 [\ a, b\ ]\right) \quad \forall x \in ([\ a, b\ ]) \quad u(a) = u(b) = 0$

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

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

$$\int_a^b \begin{matrix} u(x)\ *\cdot P(x)\cdot\frac{\partial^2}{\partial x^2}\ v(x)\ ... \\ + u(x)\ *\cdot R(x)\cdot\frac{\partial}{\partial x}\ v(x)\ ... \\ + u(x)\ *\cdot Q(x)\cdot v(x) \end{matrix}\ dx = \int_a^b u(x)\ *\cdot\begin{pmatrix} P(x)\cdot\frac{\partial^2}{\partial x^2}\ ... \\ + 2\cdot\frac{\partial}{\partial x}P(x)\cdot\frac{\partial}{\partial x}\ ... \\ + \frac{\partial^2}{\partial x^2}P(x)\ ... \\ + R(x)\cdot\frac{\partial}{\partial x} + \frac{\partial}{\partial x}R(x) + Q(x) \end{pmatrix}\cdot v(x)\ dx = \int_a^b u(x)\ *\ \mathbf{A_x}^{\dagger}\ v(x)\ dx$$

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

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

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

Example Adj$_3$)

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

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

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

$$\text{resulting adjoint operator}\ \mathbf{A}^{\dagger} = P(x)\cdot\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x}P(x)\cdot\frac{\partial}{\partial x} + Q(x) = P(x)\cdot\frac{\partial^2}{\partial x^2} + R(x)\cdot\frac{\partial}{\partial x} + Q(x) = \mathbf{A}$$

$$\text{If}\ \ R(x) = \frac{\partial}{\partial x}P(x) \ \Rightarrow\ \ \mathbf{A}^{\dagger} = \mathbf{A}$$

Example Adj$_4$)

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

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

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

Example Adj$_5$)

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

$$\text{with}\quad \boxed{P(x) = 1}\quad \boxed{R(x) = 0}\quad \boxed{Q(x) = 0}$$

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

$$\text{resulting adjoint operator}\qquad \mathbf{A} = \frac{\partial^2}{\partial x^2} \quad\Rightarrow\quad \mathbf{A}^{\dagger} = \frac{\partial^2}{\partial x^2} \quad\Rightarrow\quad \mathbf{A}^{\dagger} = \mathbf{A}$$

Example Adj$_6$)

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

$$\text{with}\quad \boxed{P(x) = 0}\quad \boxed{R(x) = 1}\quad \boxed{Q(x) = 0}$$

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

$$\text{resulting adjoint operator}\qquad \mathbf{A} = \frac{\partial}{\partial x} \quad\Rightarrow\quad \mathbf{A}^{\dagger} = -\frac{\partial}{\partial x}$$

Example Adj$_7$)

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

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

with $\boxed{P(x) = 0}$ $\boxed{R(x) = -i}$ $\boxed{Q(x) = 0}$

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

resulting adjoint operator $\mathbf{A} = -i\cdot\frac{\partial}{\partial x} \Rightarrow \mathbf{A}^{\dagger} = i\cdot\frac{\partial}{\partial x}$

Example Adj$_8$)

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

$\boxed{P(x) = -1}$ $\boxed{R(x) = 0}$ $\boxed{Q(x) = 0}$

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

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

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

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

Example Adj$_9$)

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

$\boxed{P(x) = 1}$ $\boxed{R(x) \neq 0}$ $\boxed{Q(x) \neq 0}$

The Wronskian is: $W(\xi) = f'_1(\xi)\cdot f_2(\xi) - f'_2(\xi)\cdot f_1(x)$

it satisfy the differential equation

$\mathbf{A_x}\, G(x,\xi) = \delta(x-\xi)$ where G(x,ξ) is the Green function:

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

For the variable ξ there is a second differential equation, namely:

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

resulting adjoint operator $\boxed{\mathbf{A}^{\dagger} = \frac{\partial^2}{\partial x^2} - R(x)\cdot\frac{\partial}{\partial x} - \frac{\partial}{\partial x}R(x) + Q(x)}$

Example Adj$_{10}$)

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

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

$$\left(\nabla^2\right)^{\dagger} = \nabla^2$$

Example Adj$_{11}$)

$$\mathbf{A} = \nabla\,\bullet = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$$

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

$$(\nabla\,\bullet)^{\dagger} = -\nabla\,\bullet$$

Example Adj$_{12}$)

$$\mathbf{A} = \nabla = \frac{\partial}{\partial x}\cdot\mathbf{i_x} + \frac{\partial}{\partial y}\cdot\mathbf{i_y} + \frac{\partial}{\partial z}\cdot\mathbf{i_z}$$

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

$$\nabla^{\dagger} = -\nabla$$

Examples of adjoint operators calculation

Example Adj13)

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 I is the identity operator and λ is 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: $(\mathbf{A} - \lambda\cdot\mathbf{I})\,|\,x> = |\,0>$ that is it must be satisfied the eigenvalue equation $\mathbf{A}\,|\,x> = \lambda\,|\,x>$.

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

Vice versa when the values of λ 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 λ belongs to the solving set of the operator **A** .
2) if the operator $(\mathbf{A} - \lambda\cdot\mathbf{I})^{-1}$ isn't limited, then λ belongs to the continuous spectrum of **A** .

Consider the space $(L = \{\,|\,x>\,\}) \in \mathbb{H}$. Each linear operator **A** has its eigenkets and the corresponding eigenvalue satisfying the equation:

$$\mathbf{A}\,|\,x> = \lambda\,|\,x>, \tag{9.1}$$

where the λ are numbers and are the eigenvalues of the operator **A**, they constitute the set of the eigenvalues of the operator **A** . To each eigenvector is associated an eigenvalue.
If there exist several linear independent eigenkets belonging to the same eigenvalue λ, any linear combination of this kets is an eigenket of **A** belonging to this λ. That is the ensemble of eigenkets of **A** belonging to λ forms a vector space called ***the subspace of the eigenvalue*** λ. 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 eigenbras and the corresponding eigenvalues of the operator **A** satisfy the equation:

$$<y\,|\,\mathbf{A} = <y\,|\,\mu, \tag{9.2}$$

where the μ are numbers and are other eigenvalues of the operator **A.** λ and μ constitutes the spectrum of **A.**

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

i) the two eigenvalues spectra are identical (λ=μ),

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

$$<x\,|\,\mathbf{A}\,|\,x>^* = <x\,|\,\mathbf{A}^{\dagger}\,|\,x> = <x\,|\,\mathbf{A}\,|\,x> = [\lambda\cdot(<x\,|\,x>)]^* = \lambda\cdot(<x\,|\,x>),$$

$<x\,|\,\mathbf{A}\,|\,x>$ and $<x\,|\,x>$ are real, therefore also λ is real.

iii) each eigenket and eigenbra correspond to the same eigenvalue λ=μ . The subspace of the eigenbras of μ is the dual space of the subspace of the eigenkets of the same eigenvalue.

iv) Eigenvectors belonging to distinct eigenvalues are orthogonal.

Given $\mathbf{A}\,|\,x> = \lambda\,|\,x>$ and $<y\,|\,\mathbf{A} = <y\,|\,\mu$, $<y\,|\,\mathbf{A}\,|\,x> = <y\,|\,\lambda\,|\,x> = \lambda\cdot(<y\,|\,x>)$,

$<y\,|\,\mathbf{A} = <y\,|\,\mu \quad <y\,|\,\mathbf{A}\,|\,x> = <y\,|\,\mu\,|\,x> = \mu\cdot(<y\,|\,x>)$,

subtracting term by term I get: $<y\,|\,\mathbf{A}\,|\,x> - <y\,|\,\mathbf{A}\,|\,x> = 0 = (\lambda - \mu)\cdot(<y\,|\,x>)$, consequently if $\lambda \neq \mu$, $<y\,|\,x> = 0$.

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 [6]

Consider the Hilbert space $\mathbb{H}$ and a subspace $\hbar \subseteq \mathbb{H}$. $\hbar$ is linear and closed. The ket $|\,x> \in \mathbb{H}$ can be divided in two vectors: $| x_s >$ and $| x_n >$, such that $| x_s > \in \mathscr{h}$ and $| x_n >$ has the property to be orthogonal to each vector of $\mathscr{h}$, that is $< x_s | x_n > = 0,\ \forall | x_s > \in \mathscr{h}$. If the space $\mathscr{h}$ is closed under multiplication by a number and under vector addition, that is if $| x >$ and $| y > \in \mathscr{h}$ and $\alpha, \beta \in \mathbb{C}$,

$$\mathbf{P}\left(\alpha | x > + \beta | y >\right) = \alpha \mathbf{P} | x > + \beta \mathbf{P} | y > = \alpha | x > + \beta | y >$$

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

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

<u>Properties:</u> **P** is limited: $\left|\mathbf{P} | x >\right| \leq \left|| x >\right|$ (10.1)

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

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

$$\mathbf{P}\,\mathbf{P} | x > = \mathbf{P} | x_s > = | x_s > \tag{10.4}$$

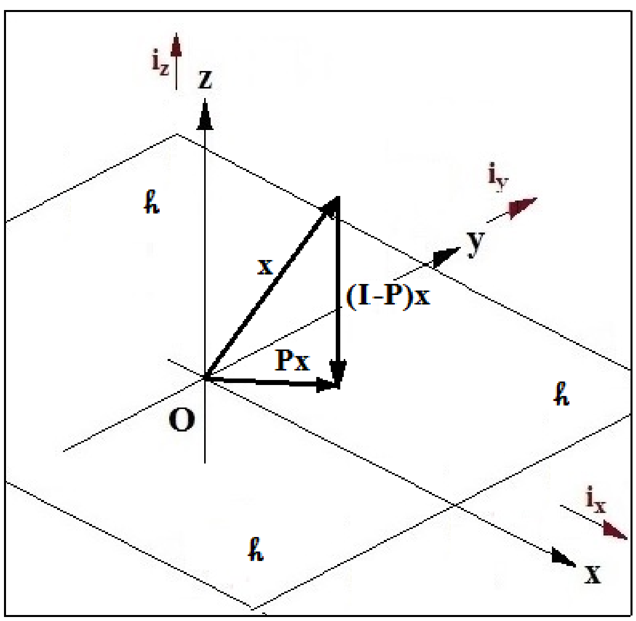
It is auto-adjunct or Hermitian: $\mathbf{P} = \mathbf{P}^{\dagger}$ necessary and sufficient condition (10.3)

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

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

$$\mathscr{h} = \mathbf{P}\,\mathbb{H}$$

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



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

The projector $\mathbf{I} - \mathbf{P}$ determines another subspace, the ortonormal one, denoted by $\mathscr{h}^{\perp}$. All vector $| x_s >$ of $\mathscr{h}$ are orthonormal to the vectors $| x_n >$ of $\mathscr{h}^{\perp}$. Then:

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

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

verify the orthonormality:

$$< x_s | x_n > = < x | \mathbf{P}(\mathbf{I} - \mathbf{P}) | x > = < x | \left(\mathbf{P} - \mathbf{P}^2\right) | x > = < x | (\mathbf{P} - \mathbf{P}) | x > = 0$$

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

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

$$\mathscr{h} = \mathscr{h}_2 \oplus \mathscr{h}_2 .$$

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

$$\mathscr{h} = \sum_j \oplus \mathscr{h}_j = \{ \sum_j | x_j > : | x_j > \in \mathscr{h}_j \}.$$

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

$$\mathrm{Tr}(\mathbf{A}) = \sum_\gamma < a_\gamma | \mathbf{A} | a_\gamma >$$

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

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

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

$$\mathbb{H} = \sum_j \oplus \mathscr{h}_j = \mathscr{h}_0 \oplus \mathscr{h}_1 \oplus \mathscr{h}_2 \oplus \mathscr{h}_3 \oplus \ldots$$

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

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

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

$$| f > = \sum_{n=0}^{\infty} \left(\mathbf{P_n} | f >\right).$$

which is equivalent writing:

$$| f > = \sum_{n=0}^{\infty} \left(| a_\gamma > < a_\gamma | f >\right)$$

Elementary projector $\quad \mathbf{P_a} = | a > < a |$ (10.5)

$$| a > < a | = \mathbf{I} \tag{10.6}$$

Given the orthonormal set $\mathscr{h}^{\perp}=\{| k >\}$ with k=1,2,...,n, $< m \left(| n >\right) = \delta_{m,n}$ (10.7)

The projector on the subset E_1 is: $P_1 = \sum_{j=1}^{N} | j >< j |$ (10.8)

If given a $| \xi >$ and ξ is continuous in (ξ_1, ξ_2), $< \xi_1 | \xi > = \Delta(\xi_1 - \xi)$ (10.9)

The projector on the subset E_2 is: $\mathbf{P_2} = \int_{\xi_1}^{\xi_2} | \xi > d\xi < \xi |$ (10.10)

degenerate spectrum $$\mathbf{P_2} | u > = \int_{\xi_1}^{\xi_2} | \xi > d\xi < \xi | u > \quad (10.11)$$

Closure relation: $$\mathbf{P_A} = \sum_{j=1}^{N} | j >< j | + \int_{\xi_1}^{\xi_2} | \xi > d\xi < \xi | = 1 \quad (10.12)$$

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

$$| \psi > = \mathbf{P_A} | \psi > = \sum_{k=1}^{N} | k >< k | \psi > + \int_{\xi_1}^{\xi_2} | \xi > d\xi < \xi | \psi >$$

Parseval $$< \psi | \psi > = < \psi | \mathbf{P_A} | \psi > = < \psi | \left(\sum_{k=1}^{N} | k >< k | + \int_{\xi_1}^{\xi_2} | \xi > d\xi < \xi | \right) | \psi >$$

$$< \psi | \psi > = \sum_{k=1}^{N} \left(|< k | \psi >| \right)^2 + \int_{\nu_1}^{\nu_2} \left(|< \nu | \psi >| \right)^2 d\nu$$

$$\mathbf{H} = \mathbf{H}\, \mathbf{P_H} = \sum_{k=1}^{N} | k > \lambda_k < k | + \int_{\nu_1}^{\nu_2} | \nu > \lambda(\nu)\, d\nu < \nu |$$

$$f(\mathbf{H}) = \sum_{k=1}^{N} | k > f(\lambda_k) < k | + \int_{\nu_1}^{\nu_2} | \nu > f(\lambda(\nu))\, d\nu < \nu |$$

11 Commutator Operator [4]

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

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

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

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

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

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

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

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

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

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

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

Momentum observables $\mathbf{p_i} = -i\cdot\hbar\cdot\dfrac{\partial}{\partial q_i}$, i=1,2,...,N, (10.11)

$$[\mathbf{q_i},\mathbf{q_j}] = 0 \qquad (10.12)$$

$$[\mathbf{p_i},\mathbf{p_j}] = 0 \qquad (10.13)$$

$$[\mathbf{q_i},\mathbf{p_j}] = i\cdot\hbar\cdot\delta(i,j) \qquad (10.14)$$

$$[\mathbf{q_i},\mathbf{F}(\mathbf{q_1},\mathbf{q_2},\ldots,\mathbf{q_n})] = 0 \qquad (10.15)$$

$$[\mathbf{p_i},\mathbf{G}(\mathbf{p_1},\mathbf{p_2},\ldots,\mathbf{p_n})] = 0 \qquad (10.16)$$

$$[\mathbf{p_i},\mathbf{F}(\mathbf{q_1},\mathbf{q_2},\ldots,\mathbf{q_n})] = -i\cdot\hbar\cdot\frac{\partial}{\partial \mathbf{q_i}}\mathbf{F} \qquad (10.17)$$

$$[\mathbf{q_i},\mathbf{G}(\mathbf{p_1},\mathbf{p_2},\ldots,\mathbf{p_n})] = i\cdot\hbar\cdot\frac{\partial}{\partial \mathbf{p_i}}\mathbf{G} \qquad (10.18)$$

$$[\mathbf{p_i},\mathbf{A}(\mathbf{p_i},\mathbf{q_i})] = -i\cdot\hbar\cdot\frac{\partial}{\partial \mathbf{q_i}}\mathbf{A}(\mathbf{p_i},\mathbf{q_i}) \qquad (10.19)$$

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

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

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

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

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

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

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

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

$$< v \mid = < u \mid \mathbf{A} \quad \Rightarrow \quad \mid v > = < v \mid * = (< u \mid \mathbf{A}) * = \mathbf{A}^{\dagger} \mid u > \tag{12.2}$$

$$< y \mid \mathbf{A} \mid x > = (< x \mid \mathbf{A}^{\dagger} \mid y >) * \tag{12.3}$$

$$\left(\mathbf{A}^{\dagger}\right)^{\dagger} = \mathbf{A} \tag{12.4}$$

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

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

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

$$(\mid u >< v \mid)^{\dagger} = \mid v >< u \mid \tag{12.8}$$

$$\text{Hermitian or self-adjoint operator: } \mathbf{A} = \mathbf{A}^{\dagger} \Rightarrow < y \mid \mathbf{A} \mid x > * = < x \mid \mathbf{A} \mid y > \tag{12.9}$$

$$\text{Anti - Hermitian operator } \mathbf{B} = -\mathbf{B}^{\dagger} \tag{12.10}$$

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

$$\mathbf{A} = \mathbf{A} + \frac{\mathbf{A}^{\dagger}}{2} - \frac{\mathbf{A}^{\dagger}}{2} = \frac{\mathbf{A}+\mathbf{A}^{\dagger}}{2} + \frac{\mathbf{A}-\mathbf{A}^{\dagger}}{2} = \mathcal{A}_{+} + \mathcal{A}_{-} \tag{12.11}$$

$$\text{Hermitian } \mathcal{A}_{+} = \frac{\mathbf{A}+\mathbf{A}^{\dagger}}{2} \qquad \mathcal{A}_{-} = \frac{\mathbf{A}-\mathbf{A}^{\dagger}}{2} \text{ anti - Hermitian} \tag{12.12}$$

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

$$\mathcal{A}_{+} = (\mathcal{A}_{+})^{\dagger} \qquad \mathcal{B}_{+} = (\mathcal{B}_{+})^{\dagger} \quad \Rightarrow \quad (\mathcal{A}_{+}\cdot\mathcal{B}_{+})^{\dagger} = (\mathcal{B}_{+})^{\dagger}\cdot(\mathcal{A}_{+})^{\dagger} = \mathcal{B}_{+}\cdot\mathcal{A}_{+} = \mathcal{A}_{+}\cdot\mathcal{B}_{+} \tag{12.14}$$

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

The commutator of two Hermitian operators is anti - Hermitian:

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

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

$$\text{two Hermitian operators } \mathcal{C}_{+} = (\mathcal{C}_{+})^{\dagger} \qquad \mathcal{D}_{+} = (\mathcal{D}_{+})^{\dagger}$$

$$[\, \mathcal{C}_{+}, \mathcal{D}_{+} \,] = \mathcal{C}_{+}\cdot\mathcal{D}_{+} - \mathcal{D}_{+}\cdot\mathcal{C}_{+} = (\mathcal{C}_{+})^{\dagger}\cdot(\mathcal{D}_{+})^{\dagger} - (\mathcal{D}_{+})^{\dagger}\cdot(\mathcal{C}_{+})^{\dagger}$$

$$(\mathcal{C}_{+})^{\dagger}\cdot(\mathcal{D}_{+})^{\dagger} - (\mathcal{D}_{+})^{\dagger}\cdot(\mathcal{C}_{+})^{\dagger} = (\mathcal{D}_{+}\cdot\mathcal{C}_{+})^{\dagger} - (\mathcal{C}_{+}\cdot\mathcal{D}_{+})^{\dagger}$$

$$(\mathcal{D}_{+}\cdot\mathcal{C}_{+})^{\dagger} - (\mathcal{C}_{+}\cdot\mathcal{D}_{+})^{\dagger} = (\mathcal{D}_{+}\cdot\mathcal{C}_{+} - \mathcal{C}_{+}\cdot\mathcal{D}_{+})^{\dagger} = -([\, \mathcal{C}_{+}, \mathcal{D}_{+} \,])^{\dagger}$$

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

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

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

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

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

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

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

Definition: $\mathbf{A}(\mathbf{B})^k = [\, \mathbf{A}, [\, \mathbf{A}, [\, \mathbf{A}, [\, \mathbf{A}, [\, \mathbf{A}, [\, \mathbf{A}, \mathbf{B} \,]\,]\,]\,]\,]\,]$ k times (12.21)

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

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

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

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

$$\mathcal{C}_{+}\cdot\mathcal{D}_{+} = \frac{\mathcal{C}_{+}\cdot\mathcal{D}_{+} + \mathcal{D}_{+}\cdot\mathcal{C}_{+}}{2} + \frac{1}{2}\cdot\left([\ \mathcal{C}_{+}, \mathcal{D}_{+}\ ]\right) \tag{13.1}$$

Particular Hermitian Operator: $|\ \mathrm{u} >< \mathrm{v}\ |$ It has no inverse. (13.2)

$$|\ \mathrm{u} >< \mathrm{v}\ |\ \mathrm{w} > = \mathrm{const}\cdot(|\ \mathrm{u} >) \tag{13.3}$$

$$< \mathrm{w}\ |\ \mathrm{v} >< \mathrm{u}\ | = \mathrm{const}\cdot(< \mathrm{v}\ |) \tag{13.4}$$

14 *Expectation value of the Operator*

$$< \mathbf{A} > = \frac{< \psi\ |\ \mathbf{A}\ |\ \psi >}{< \psi\ |\ \psi >} = \frac{\int \Psi(\tau)^{*}\cdot\mathbf{A}\cdot\Psi(\tau)\, d\tau}{\int \Psi(\tau)^{*}\cdot\Psi(\tau)\, d\tau} \tag{14.1}$$

for normalized eigenfunction: $< \psi\ |\ \psi > = 1$

$$< \mathbf{A} > = < \psi\ |\ \mathbf{A}\ |\ \psi > = \int \Psi(\tau)^{*}\cdot\mathbf{A}\cdot\Psi(\tau)\, d\tau \tag{14.2}$$

$$< \mathrm{F}(\mathbf{A}) > = \sum_{n} \mathrm{P_n}\left(< \mathrm{n}\ |\ \mathbf{F}(\mathbf{A})\ |\ \mathrm{n} >\right) \tag{14.3}$$

$$\Delta\,\mathbf{A} = \sqrt{< (\mathbf{A} - < \mathbf{A} >)^{2} >} \tag{14.4}$$

$$< \mathbf{A} - \mathbf{B} > = < \mathbf{A} > - < \mathbf{B} > \tag{14.5}$$

15 *Heisenberg uncertainty principle*

$$\Delta\,\mathbf{A}\cdot\Delta\,\mathbf{B} \geq \frac{1}{2}\cdot\left|< [\ \mathbf{A}, \mathbf{B}\ ] >\right| \tag{15.1}$$

Demonstration of 15.1)

$$\Delta\,\mathbf{A} = \sqrt{< (\mathbf{A} - < \mathbf{A} >)^{2} >} = \sqrt{< \mathbf{A}^{2} > - (< \mathbf{A} >)^{2}}$$

$$\mathbf{A_1} = \mathbf{A} - < \mathbf{A} >$$

$$\Delta\,\mathbf{A} = \sqrt{< \mathbf{A_1}^{2} >}$$

$$\Delta\,\mathbf{B} = \sqrt{< (\mathbf{B} - < \mathbf{B} >)^{2} >} = \sqrt{< \mathbf{B}^{2} > - (< \mathbf{B} >)^{2}}$$

$$\mathbf{B_1} = \mathbf{B} - < \mathbf{B} >$$

$$\Delta\,\mathbf{B} = \sqrt{< \mathbf{B_1}^{2} >}$$

$$(\Delta A \cdot \Delta B)^2 = \left(< A_1{}^2 >\right)\cdot\left(< B_1{}^2 >\right) = < \psi \mid A_1{}^2 \mid \psi > \cdot < \psi \mid B_1{}^2 \mid \psi >$$

Self adjoint Operators (Hermitian)

$$A_1 = A_1{}^{\dagger} \qquad B_1 = B_1{}^{\dagger}$$

$$< \psi \mid A_1{}^2 \mid \psi > \cdot < \psi \mid B_1{}^2 \mid \psi > = < \psi \mid A_1 \cdot A_1 \mid \psi > \cdot < \psi \mid B_1 \cdot B_1 \mid \psi >$$

$$\mid z > = A_1 \mid \psi > \qquad \mid \zeta > = B_1 \mid \psi >$$

$$< \psi \mid A_1 \cdot A_1 \mid \psi > \cdot < \psi \mid B_1 \cdot B_1 \mid \psi > = < \psi \mid A_1 \mid z > \cdot < \psi \mid B_1 \mid \zeta >$$

$$< \psi \mid A_1 \mid z > = < z \mid A_1 \mid \psi > * = < z \mid z > * = \left(\left|A_1 \mid \psi >\right|\right)^2$$

$$< \psi \mid B_1 \mid \zeta > = < \zeta \mid B_1 \mid \psi > * = < \zeta \mid \zeta > * = \left(\left|B_1 \mid \psi >\right|\right)^2$$

$$(\Delta A \cdot \Delta B)^2 = < \psi \mid A_1 \mid z > \cdot < \psi \mid B_1 \mid \zeta > = \left(\left|A_1 \mid \psi >\right|\right)^2 \cdot \left(\left|B_1 \mid \psi >\right|\right)^2$$

Schwarz inequality $$\left(\left|< x \mid A \mid y >\right|\right)^2 \le < x \mid A \mid x > \cdot \left(< y \mid A \mid y >\right) \qquad (5.13')$$

$$(\Delta A \cdot \Delta B)^2 = \left(\left|A_1 \mid \psi >\right|\right)^2 \cdot \left(\left|B_1 \mid \psi >\right|\right)^2 = < \psi \mid A_1 \mid z > \cdot < \psi \mid B_1 \mid \zeta > \ge \left(\left|< \psi \mid A_1 \cdot B_1 \mid \psi >\right|\right)^2$$

$$(\Delta A \cdot \Delta B)^2 \ge \left(\left|< \psi \mid A_1 \cdot B_1 \mid \psi >\right|\right)^2$$

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

$$\left(A_1 \cdot B_1\right)^{\dagger} = \left(B_1\right)^{\dagger} \cdot A_1{}^{\dagger} = B_1 \cdot A_1$$

$$(\Delta A \cdot \Delta B)^2 \ge \left[\left|< \psi \mid \left(\frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} + \frac{[\, A_1 , B_1 \,]}{2}\right) \mid \psi >\right|\right]^2$$

$$(\Delta A \cdot \Delta B)^2 \ge \left(\left|< \psi \mid \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} \mid \psi > + < \psi \mid \frac{[\, A_1 , B_1 \,]}{2} \mid \psi >\right|\right)^2$$

$$< \psi \mid \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} \mid \psi > = < \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} >$$

$$< \psi \mid \frac{[\, A_1 , B_1 \,]}{2} \mid \psi > = < \frac{[\, A_1 , B_1 \,]}{2} >$$

$$(\Delta A \cdot \Delta B)^2 \ge \left(\left|< \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} > + < \frac{[\, A_1 , B_1 \,]}{2} >\right|\right)^2$$

assuming that the average $< \dfrac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} >$ is real and $< \dfrac{[\, A_1 , B_1 \,]}{2} >$ is imaginary, I get:

$$< \frac{A_1 \cdot B_1 + B_1 \cdot A_1}{2} > = < \psi \mid \frac{A_1 \cdot B_1}{2} \mid \psi > \dots$$

$$+ < \psi \mid \frac{B_1 \cdot A_1}{2} \mid \psi >$$

$$A_1 = c \cdot B_1$$

$$< \psi \mid \frac{\alpha^* \cdot B_1 \cdot B_1}{2} \mid \psi > \dots = (\alpha^* + \alpha) \cdot < \psi \mid \frac{B_1 \cdot B_1}{2} \mid \psi > = \mathrm{Re}(\alpha) \cdot < \psi \mid \frac{{B_1}^2}{2} \mid \psi >$$

$$+ < \psi \mid \frac{\alpha \cdot B_1 \cdot B_1}{2} \mid \psi >$$

$$\mathrm{Re}(\alpha) \cdot < \psi \mid \frac{{B_1}^2}{2} \mid \psi > = 0 \qquad \text{if} \quad \mathrm{Re}(\alpha) = 0$$

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

The minimum for $\Delta A \cdot \Delta B$ is reached when

$$< A_1 \cdot B_1 + B_1 \cdot A_1 > = 0 \qquad \text{finally resulting:}$$

$$A_1 = A - < A >$$

$$B_1 = B - < B >$$

$$[\, A_1 , B_1 \,] = A_1 \cdot B_1 - B_1 \cdot A_1 = (A - < A >) \cdot (B - < B >) - (B - < B >) \cdot (A - < A >)$$

$$(A - < A >) \cdot (B - < B >) \dots \qquad = A \cdot B - A \cdot (< B >) - (< A >) \cdot B + (< A >) \cdot (< B >) \dots$$

$$+ (-1) \cdot [(B - < B >) \cdot (A - < A >)] \qquad + (-1) \cdot [B \cdot A - B \cdot (< A >) - (< B >) \cdot A + (< B >) \cdot (< A >)]$$

$$A \cdot B - A \cdot (< B >) - (< A >) \cdot B + (< A >) \cdot (< B >) - B \cdot A + B \cdot (< A >) + (< B >) \cdot A - (< B >) \cdot (< A >)$$

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

$$\Delta A \cdot \Delta B \geq \frac{1}{2} \cdot \left| < [\, A_1 , B_1 \,] > \right| = \frac{1}{2} \cdot \left| < [\, A , B \,] > \right|$$

$$\boxed{\Delta A \cdot \Delta B \geq \frac{1}{2} \cdot \left| < [\, A , B \,] > \right|}$$

Demonstration of 15.1)

16 Wave Mechanics [3]

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 ant kinetic energy $T_p = \frac{p^2}{2 \cdot m_p}$. Than I can write $p = \sqrt{2 \cdot m_p \cdot T_p}$ and since $p = \hbar \cdot k_p$, where $k_p = \frac{2 \cdot \pi}{\lambda_p}$, results the wavelength of the particle $\boxed{\lambda_p = \frac{2 \cdot \pi \cdot \hbar}{\sqrt{2 \cdot m_p \cdot T_p}} = \frac{h}{\sqrt{2 \cdot m_p \cdot T_p}}}$ which is the known de Broglie wavelength of the particle. For example if $m_p := m_e$ and $T_{p1} := 1 \cdot eV$, the de Broglie wavelength is $\lambda_e := \frac{h}{\sqrt{2 \cdot m_p \cdot T_{p1}}} = 12.265 \cdot Å$ so that if $T_p = z_p \cdot T_{p1}$ with $z_p := 5 \cdot 10^4$ than $\lambda_p := \frac{12.265\ Å}{\sqrt{z_p}}$ that is $\lambda_p = 0.055 \cdot Å$

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

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

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:

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

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

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:

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

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

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

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 Δk around k_1.The wave is concentrate in a region $\Delta x \approx \left(\frac{1}{\Delta k_1}\right)$, where

$$\frac{\partial}{\partial k_1}\varphi(k_1) = x - t \cdot \frac{\partial}{\partial k_1}\omega(k_1) + \frac{\partial}{\partial k_1}\alpha(k_1) = 0, \text{ namely} \tag{16.5}$$

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

with a velocity:

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

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

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

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

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

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

Postulates

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

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

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

This is a solution of the differential equation:

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

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

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

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

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

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

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

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

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

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

Schrödinger equation ([4] Vol. I)

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

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

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

where $\mathbf{p} = p_x\cdot\mathbf{i_x} + p_y\cdot\mathbf{i_y} + p_z\cdot\mathbf{i_z}$ $\qquad$ $\mathbf{r} = x\cdot\mathbf{i_x} + y\cdot\mathbf{i_y} + z\cdot\mathbf{i_z}$ $\qquad$ 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:

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

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

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

Now calculate the gradient of 16.23):

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

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

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

Than the divergence of it:

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

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

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

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

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

$$i\cdot\hbar\cdot\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \int \Phi(\mathbf{p})\cdot E\cdot e^{i\cdot\left(\frac{\mathbf{p}\cdot\mathbf{r}-E\cdot t}{\hbar}\right)}\,d\mathbf{p} \qquad 16.26')$$

equating 16.26') and eq 16.31) I get: $\boxed{i\cdot\hbar\cdot\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \frac{-\hbar^2}{2\cdot m}\cdot\Delta\,\Psi(\mathbf{r},t)}$

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

Laplace transform of the Schrödinger equation :

$$|\,\Psi(x,s)\,> = \mathcal{L}(|\,\psi(x,t)\,>)$$

$$\boxed{j\cdot\hbar\cdot\left[s\cdot(|\,\Psi(x,s)\,>) - |\,\psi(0)\,>\right] = \mathbf{H}\,|\,\Psi(x,s)\,>} \qquad 16.32)$$

Schrödinger equation ([4] Vol. I)

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

To solve the one-dimensional Schrödinger equation for a free particle of mass m moving with velocity v, I can proceed a follows:

Configuration space representation: $\boxed{\frac{-\hbar^2}{2\cdot m_e}\cdot\frac{\partial^2}{\partial x^2}\Psi = i\cdot\hbar\cdot\frac{\partial}{\partial t}\Psi}$ (16.33)

It allows factorization (separable variables): $\boxed{\Psi = g(t)\cdot\varphi(x)}$ (16.34)

Replacing (16.13) in (16.12) I have: $g(t)\cdot\frac{-\hbar^2}{2\cdot m_e}\cdot\frac{\partial^2}{\partial x^2}\varphi(x) = i\cdot\hbar\cdot\left(\frac{d}{dt}g(t)\right)\cdot\varphi(x)$ (16.35)

let's me put: $i\cdot\hbar\cdot\frac{d}{dt}g(t) = \hbar\cdot\omega\,g(t)$

$$\frac{-\hbar^2}{2\cdot m_e}\cdot\frac{\partial^2}{\partial x^2}\varphi(x) = \hbar\cdot\omega\,\varphi(x)$$

The equation breaks down in two differential equations:

$$\text{a)}\qquad \frac{d}{dt}g(t) = -i\cdot\omega\,g(t) \tag{16.36}$$

with solution:

$$g(t) = e^{-i\cdot\omega\cdot t} \tag{16.37}$$

and the equation:

$$\text{b)}\qquad \frac{d^2}{dx^2}\varphi(x) + \frac{2\cdot m_e\cdot\omega}{\hbar}\varphi(x) = 0 \tag{16.38}$$

If $\boldsymbol{\omega}$ is real, the solution is periodic in time, and $(\varphi(x))^2$ is independent of time (stationary case); with ω positive,

$$\frac{d^2}{dx^2}\varphi(x) + k^2\cdot(\varphi(x)) = 0 \tag{16.38'}$$

$$k^2 = \frac{2\cdot m_e\cdot\omega}{\hbar}$$

Even the constant k^2 is positive and the solutions of (16.38') are periodic even in space.
It is an essential feature of quantum mechanics that temporal dependence is of complex form (16.37).
Real sinus and cosine functions are not solutions of the differential equation (16.36). This behavior, so different from classical physics, is a consequence of Schrödinger's equation that is of first order over time.
The physical meaning of the parameter ω can be further interpreted considering the operator at the first member of (16.33) as the Hamiltonian constituted, in our case, only by the kinetic energy operator.
It follows that the kinetic energy of the particle must be real and positive. Our solution is therefore a Hamiltonian auto state. Since k^2 is a positive constant, the complete solution of (16.37') or

$$\boldsymbol{\varphi}''+k^2\boldsymbol{\varphi}=0 \tag{16.39}$$

is:

$$\varphi(x) = A\cdot\exp(i\cdot k\cdot x) + B\cdot\exp(-i\cdot k\cdot x)$$

so that the one-dimensional wave function is the product (16.34), that is:

$$\boxed{\psi(x) = A\cdot e^{i\cdot(k\cdot x-\omega\cdot t)} + B\cdot e^{-i\cdot(k\cdot x+\omega\cdot t)}} \tag{16.40}$$

consists of two waves propagating in opposite directions, both with phase velocities:

$$v_{ph} = \frac{\omega}{k}$$

The physical meaning of the spatial part of the wave function (16.40) becomes clear in obtaining the probability density
The two waves, of amplitudes A and B, apparently correspond to two opposite currents whose intensities are given by their normalization constants and is proportional to k. Density shows the interference of the two waves (consistent) causing spatial periodicity.
As long as there is no particular reason to achieve consistency (such as contour conditions), it will be reasonable to consider the two waves, put B = 0 and get s> 0, or A = 0, which provides s <0. The result thus corresponds to the linea motion of a particle in either direction. Assuming both signs of k, I can summarize the final results as follows:

$$\rho = \psi(x)\cdot\psi(x)^* \tag{16.41}$$

and the flux

$$S = \frac{\hbar}{2\cdot i\cdot m_e}\cdot\left(\psi(x)^*\cdot\frac{\partial}{\partial x}\psi(x) - \psi(x)\cdot\frac{\partial}{\partial x}\psi(x)^*\right) \tag{16.42}$$

finding that:

$$\rho = (|A|)^2 + (|B|)^2 + \left(A\cdot B^*\cdot e^{2\cdot i\cdot k\cdot x} + A^*\cdot B\cdot e^{-2\cdot i\cdot k\cdot x}\right)$$

$$E = \hbar\cdot\omega \qquad k^2 = \frac{2\cdot m_e\cdot\omega}{\hbar} \qquad E = \frac{\hbar^2\cdot k^2}{2\cdot m_e} \tag{16.43}$$

$$S = \frac{\hbar\cdot k}{m_e}\cdot\left[(|A|)^2 - (|B|)^2\right] \tag{16.44}$$

$$\rho = (|C0(k)|)^2 \qquad s_0 = \frac{\hbar\cdot k}{m_e}\cdot(|C0(k)|)^2$$

$$\Psi(x,t) = C0(k)\cdot e^{i\cdot(k\cdot x-\omega\cdot t)} \tag{16.45}$$

$$p(k) = \hbar\cdot k \qquad v(k) = \frac{\hbar\cdot k}{m_e}$$

$$\Psi(x,t) = C0(k)\cdot e^{i\cdot k\cdot t\cdot\left(v-v_{ph}\right)}$$

The latter is different from the phase velocity of the wave:

$$v_{ph}(\omega,k) := \frac{\omega(k)}{k}$$

$$\frac{\omega(k)}{k} = \frac{E(k)}{p(k)}$$

$$\frac{E(k)}{p(k)} = \frac{v_{ph}(k)}{2}$$

and it is identical to the group velocity: $v_{gr}(k,\omega) = \frac{\partial}{\partial k}\omega$

$$\frac{\partial}{\partial k}\omega(k) = \frac{\partial}{\partial p}E(k)$$

$$v = \frac{\partial}{\partial p}E(k)$$

I have seen that:

$$\Psi(x,t) = C0(k)\cdot\exp\left[i\cdot(k\cdot x - \omega\cdot t)\right] = C0(k)\cdot e^{i\cdot\left[k\cdot t\cdot\left(v-v_{ph}\right)\right]} \tag{16.46}$$

$$\omega(k) := \frac{\hbar}{2\cdot m_e}\cdot k^2 \tag{16.47}$$

k is an independent variable, so that the complete solution of the equation is obtained by integrating on k:

$$k_0 = \frac{m_e\cdot v}{\hbar} \qquad \Psi(x,0) = A\cdot\exp\left(\frac{-x^2}{2\cdot a^2} + i\cdot k_0\cdot x\right) \tag{16.48}$$

$$\Psi(x,t) = \int_{-\infty}^{\infty}\psi(k,x,t)\,dk \tag{16.49}$$

So the density: $\rho(x,0) = (|\Psi(x,0)|)^2 \qquad (|\Psi(x,0)|)^2 = (|A|)^2\cdot\exp\left(\frac{-x^2}{a^2}\right)$

locate the particle within $|x| \le a$, the flux (16.42) is:

$$s_0(x,0) = \frac{\hbar}{2\cdot m\cdot i}\cdot 2\cdot i\cdot k_0\cdot(|A|)^2\cdot\exp\left(\frac{-x^2}{a^2}\right)$$

$$s_0(x,0) = \rho\cdot\frac{\hbar}{m_e}\cdot k_0$$

so that the velocity of the particle and the moment are:

$$v_0 = \frac{\hbar}{m_e}\cdot k_0$$

$$p_0 = \hbar\cdot k_0$$

Thanks to the normalization condition:

$$\int_{-\infty}^{\infty}\rho(x)\,dx = 1$$

I get: $$(|A|)^2 = \frac{1}{a\cdot\sqrt{\pi}} \qquad |A| = \frac{1}{\sqrt{a\cdot\sqrt{\pi}}} \qquad (16.50)$$

The expression (16.48) can be decomposed into plane waves using (16.49) and (16.43)

$$\Psi(x,0) = \int_{-\infty}^{\infty} C0(k)\cdot e^{i\cdot k\cdot x}\,dx \qquad (16.51)$$

This is a Fourier integral whose inversion is:

$$C0(k) = \frac{1}{2\cdot\pi}\cdot\int_{-\infty}^{\infty}\Psi(x,0)\cdot e^{-i\cdot k\cdot x}\,dx$$

$$C0(k) = \frac{A}{2\cdot\pi}\cdot\int_{-\infty}^{\infty}\exp\left[\frac{-x^2}{2\cdot a}+i\cdot(k_0-k)\cdot x\right]dx$$

since $\int_{-\infty}^{\infty} e^{-z^2}\,dz = \sqrt{\pi}$ results: $$\boxed{C0(k) = \frac{A\cdot a}{\sqrt{2\cdot\pi}}\cdot\exp\left[\frac{-1}{2}\cdot a^2\cdot(k-k_0)^2\right]} \qquad (16.52)$$

Which can be easily understood in terms of Heisenberg's uncertainty relationship: in the initial state, the uncertainty o particle coordinate, in accordance with (16.48), of the order of **Δx** = a; as shown in (16.1), contributes to this wave function a spectrum of wave numbers k or of momentum p = $\hbar$k around k = k_0 of a width **Δ**k = 1 / a_o or **Δ**p = $\hbar$ / a. So, regardless of the choice of a, it is the relation **Δ**x **Δ**p = $\hbar$ which is the uncertainty principle of of Heisenberg.
After determining C (k) from the initial state at time t = 0, I am now ready to evaluate the integral (16.49) at any insta that is:

$$(|A|)^2 = \frac{1}{a\cdot\sqrt{\pi}} \qquad |A| = \frac{1}{\sqrt{a\cdot\sqrt{\pi}}}$$

$$\boxed{\Psi(x,t) = \frac{A\cdot a}{\sqrt{2\cdot\pi}}\cdot\int_{-\infty}^{\infty}\exp\left[\frac{-1}{2}\cdot a^2\cdot(k-k_0)^2+i\cdot k\cdot x-\frac{i\cdot\hbar\cdot t}{2\cdot m_e}\cdot k^2\right]dk} \qquad 16.53)$$

The exponent is a quadratic form in k so that, again, I can use the integral error. It is:

$$\Psi(x,t) = \frac{A\cdot a}{\sqrt{2\cdot\pi}}\cdot\int_{-\infty}^{\infty} e^{\left(-\frac{a^2}{2}-\frac{t\cdot\hbar\cdot i}{2\cdot m_e}\right)\cdot k^2+\left(k_0\cdot a^2+x\cdot i\right)\cdot k-\frac{a^2\cdot k_0{}^2}{2}}\,dk$$

(MATHCAD symbolic initialization) $t := t$ $\quad a := a$ $\quad k := k$ $\quad k_0 := k_0$ $\quad m_e := m_e$ $\quad x := x$ $\quad \hbar := \hbar$

$$\Psi(x,t) = \frac{A\cdot a\cdot e^{-\frac{a^2\cdot k_0{}^2}{2}}}{\sqrt{2\cdot\pi}}\cdot\int_{-\infty}^{\infty} e^{\left(-\frac{a^2}{2}-\frac{t\cdot\hbar\cdot i}{2\cdot m_e}\right)\cdot k^2+\left(k_0\cdot a^2+x\cdot i\right)\cdot k}\,dk$$

$$A_0 = \left(-\frac{a^2}{2}-\frac{t\cdot\hbar\cdot i}{2\cdot m_e}\right) \qquad B_0 = \left(k_0\cdot a^2+x\cdot i\right) \qquad C_0 = \frac{A\cdot a\cdot e^{-\frac{a^2\cdot k_0{}^2}{2}}}{\sqrt{2\cdot\pi}}$$

$$\boxed{\Psi(x,t) = C_0\cdot\int_{-\infty}^{\infty} e^{A_0\cdot k^2+B_0\cdot k}\,dk} \tag{16.54)}$$

$$C_0\cdot\int_{-\infty}^{\infty} e^{A_0\cdot k^2+B_0\cdot k}\,dk = \frac{\sqrt{-\pi}\cdot C_0\cdot e^{-\frac{B_0{}^2}{4\cdot A_0}}\cdot\left[\left[\lim_{k\to-\infty^+}\operatorname{erf}\left[\frac{\left(B_0+2\cdot A_0\cdot k\right)\cdot i}{2\cdot\sqrt{A_0}}\right]\right]\ldots\atop +(-1)\cdot\lim_{k\to\infty^-}\operatorname{erf}\left(\frac{\frac{1}{\sqrt{A_0}}\cdot B_0}{2}\cdot i+\sqrt{A_0}\cdot k\cdot i\right)\right]}{2\cdot\sqrt{A_0}}$$

$$\Psi(x,t) = \frac{\sqrt{-\pi}\cdot C_0\cdot e^{-\frac{B_0{}^2}{4\cdot A_0}}\cdot\left[\lim_{k\to-\infty^+}\operatorname{erf}\left[\frac{\left(B_0+2\cdot A_0\cdot k\right)\cdot i}{2\cdot\sqrt{A_0}}\right]-\lim_{k\to\infty^-}\operatorname{erf}\left(\frac{\frac{1}{\sqrt{A_0}}\cdot B_0}{2}\cdot i+\sqrt{A_0}\cdot k\cdot i\right)\right]}{2\cdot\sqrt{A_0}}$$

$$\lim_{k\to-\infty^+}\operatorname{erf}\left[\frac{\left(B_0+2\cdot A_0\cdot k\right)\cdot i}{2\cdot\sqrt{A_0}}\right] = \operatorname{erf}\left(\frac{B_0\cdot i}{2\cdot\sqrt{A_0}}\right)+\lim_{k\to-\infty^+}\operatorname{erf}\left(\sqrt{A_0}\cdot k\cdot i\right)$$

$$\lim_{k\to-\infty^+}\operatorname{erf}\left(\sqrt{A_0}\cdot k\cdot i\right) = \frac{e^{A_0\cdot k^2}}{\sqrt{A_0}}\cdot\left(\frac{i}{\sqrt{\pi}\cdot k}+\frac{i}{2\cdot A_0\cdot\sqrt{\pi}\cdot k^3}+\frac{3i}{4A_0{}^2\cdot\sqrt{\pi}\cdot k^5}\right)+i\cdot\frac{\sqrt{-A_0}}{\sqrt{A_0}}$$

$$\lim_{k\to\infty^-}\operatorname{erf}\left(\frac{\frac{1}{\sqrt{A_0}}\cdot B_0}{2}\cdot i+\sqrt{A_0}\cdot k\cdot i\right) = \operatorname{erf}\left(\frac{i\cdot B_0}{2\cdot\sqrt{A_0}}\right)+\lim_{k\to\infty}\operatorname{erf}\left(\sqrt{A_0}\cdot k\cdot i\right)$$

$$\lim_{k \to \infty} \operatorname{erf}\left(\sqrt{A_0}\cdot k\cdot i\right) = \frac{e^{A_0\cdot k^2}}{\sqrt{A_0}}\cdot\left(\frac{i}{\sqrt{\pi}\cdot k} + \frac{i}{2\cdot A_0\cdot\sqrt{\pi}\cdot k^3} + \frac{3i}{4A_0{}^2\cdot\sqrt{\pi}\cdot k^5}\right) - i\cdot\frac{\sqrt{-A_0}}{\sqrt{A_0}}$$

$$\Psi(x,t) = \frac{\sqrt{-\pi}\cdot C_0\cdot e^{-\frac{B_0{}^2}{4\cdot A_0}}\cdot\left[\operatorname{erf}\left(\frac{B_0\cdot i}{2\cdot\sqrt{A_0}}\right) \ldots + \lim_{k \to -\infty^+} \operatorname{erf}\left(\sqrt{A_0}\cdot k\cdot i\right) - \left(\operatorname{erf}\left(\frac{i\cdot B_0}{2\cdot\sqrt{A_0}}\right) + \lim_{k \to \infty} \operatorname{erf}\left(\sqrt{A_0}\cdot k\cdot i\right)\right)\right]}{2\cdot\sqrt{A_0}}$$

$$\Psi(x,t) = \frac{\sqrt{-\pi}\cdot C_0\cdot e^{-\frac{B_0{}^2}{4\cdot A_0}}\cdot\left[\operatorname{erf}\left(\frac{B_0\cdot i}{2\cdot\sqrt{A_0}}\right) + \frac{e^{A_0\cdot k^2}}{\sqrt{A_0}}\cdot\left(\frac{i}{\sqrt{\pi}\cdot k} + \frac{i}{2\cdot A_0\cdot\sqrt{\pi}\cdot k^3} + \frac{3i}{4A_0{}^2\cdot\sqrt{\pi}\cdot k^5}\right) - 1 \ldots + (-1)\cdot\left[\operatorname{erf}\left(\frac{i\cdot B_0}{2\cdot\sqrt{A_0}}\right) + \left[\frac{e^{A_0\cdot k^2}}{\sqrt{A_0}}\cdot\left(\frac{i}{\sqrt{\pi}\cdot k} + \frac{i}{2\cdot A_0\cdot\sqrt{\pi}\cdot k^3} + \frac{3i}{4A_0{}^2\cdot\sqrt{\pi}\cdot k^5}\right) + 1\right]\right]\right]}{2\cdot\sqrt{A_0}}$$

$$\Psi(x,t) = \frac{\sqrt{\pi}\cdot C_0\cdot e^{-\frac{B_0{}^2}{4\cdot A_0}}}{\sqrt{-A_0}} = \frac{\sqrt{\pi}\cdot\frac{A\cdot a\cdot e^{-\frac{a^2\cdot k_0{}^2}{2}}}{\sqrt{2\cdot\pi}}\cdot e^{-\frac{\left(k_0\cdot a^2+x\cdot i\right)^2}{4\cdot\left(-\frac{a^2}{2}-\frac{t\cdot\hbar\cdot i}{2\cdot m_e}\right)}}}{\sqrt{-\left(-\frac{a^2}{2}-\frac{t\cdot\hbar\cdot i}{2\cdot m_e}\right)}}$$

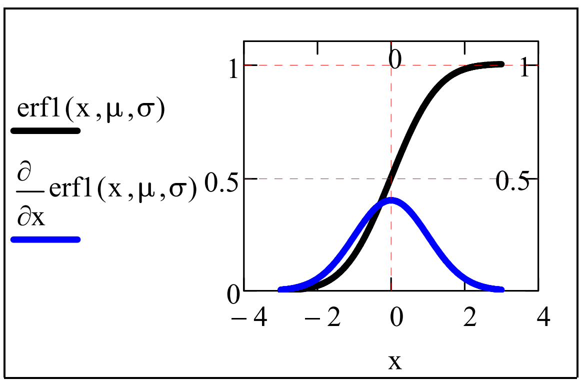
$$\Psi(x,t) = \frac{\sqrt{\pi}\cdot\frac{A\cdot a\cdot e^{-\frac{a^2\cdot k_0{}^2}{2}}}{\sqrt{2\cdot\pi}}\cdot e^{-\frac{\left(k_0\cdot a^2+x\cdot i\right)^2}{4\cdot\left(-\frac{a^2}{2}-\frac{t\cdot\hbar\cdot i}{2\cdot m_e}\right)}}}{\sqrt{-\left(-\frac{a^2}{2}-\frac{t\cdot\hbar\cdot i}{2\cdot m_e}\right)}} = \frac{A\cdot e^{-\frac{a^2\cdot k_0{}^2}{2}}\cdot e^{-\frac{\left(k_0\cdot a^2+x\cdot i\right)^2}{4\cdot\left(-\frac{a^2}{2}-\frac{t\cdot\hbar\cdot i}{2\cdot m_e}\right)}}}{\sqrt{1+\frac{t\cdot\hbar\cdot i}{m_e\cdot a^2}}}$$

$$\frac{A\cdot e^{-\frac{a^2\cdot k_0^{\,2}}{2}}\cdot e^{-\frac{\left(k_0\cdot a^2+x\cdot i\right)^2}{4\cdot\left(-\frac{a^2}{2}-\frac{t\cdot\hbar\cdot i}{2\cdot m_e}\right)}}}{\sqrt{1+\frac{t\cdot\hbar\cdot i}{m_e\cdot a^2}}} = \frac{A\cdot e^{\frac{\left(2\cdot m_e\cdot a^2\cdot k_0\cdot x-t\cdot\hbar\cdot a^2\cdot k_0^{\,2}+m_e\cdot x^2\cdot i\right)\cdot i}{2\cdot\left(m_e\cdot a^2+t\cdot\hbar\cdot i\right)}}}{\sqrt{1+\frac{t\cdot\hbar\cdot i}{m_e\cdot a^2}}} = \frac{A\cdot e^{\frac{\left(k_0\cdot x-\frac{t\cdot\hbar\cdot k_0^{\,2}}{2\cdot m_e}+\frac{x^2}{2\cdot a^2}\cdot i\right)\cdot i}{\left(1+\frac{t\cdot\hbar\cdot i}{m_e\cdot a^2}\right)}}}{\sqrt{1+\frac{t\cdot\hbar\cdot i}{m_e\cdot a^2}}}$$

$$\mathrm{erf1}(x,\mu,\sigma) := \frac{1}{\sqrt{2\cdot\pi}}\cdot\int_{-\infty}^{x} e^{-\frac{\xi^2}{2}}\,d\xi$$

$$\mu := 0.3 \qquad \sigma := 0.3$$

$$x := -10\cdot\sigma, -10\cdot\sigma+\frac{20\cdot\sigma}{1000}\,..\,10\cdot\sigma$$



$$\Psi(x,t) = \frac{A}{\sqrt{1+\frac{i\cdot\hbar\cdot t}{m_e\cdot a^2}}}\cdot\exp\left[\frac{-\left(x^2-2\cdot i\cdot a^2\cdot k_0\cdot x+\frac{i\cdot\hbar\cdot t}{2\cdot m_e}\cdot k_0^{\,2}\cdot a^2\right)}{2\cdot a^2\cdot\left(1+\frac{i\cdot\hbar\cdot t}{m_e\cdot a^2}\right)}\right] \tag{16.55}$$

Let's say, for example: $v := 10^3\cdot\frac{m}{s}$ $\quad a := 10^{-6}\cdot m$ $\quad$ and that|A|=A:

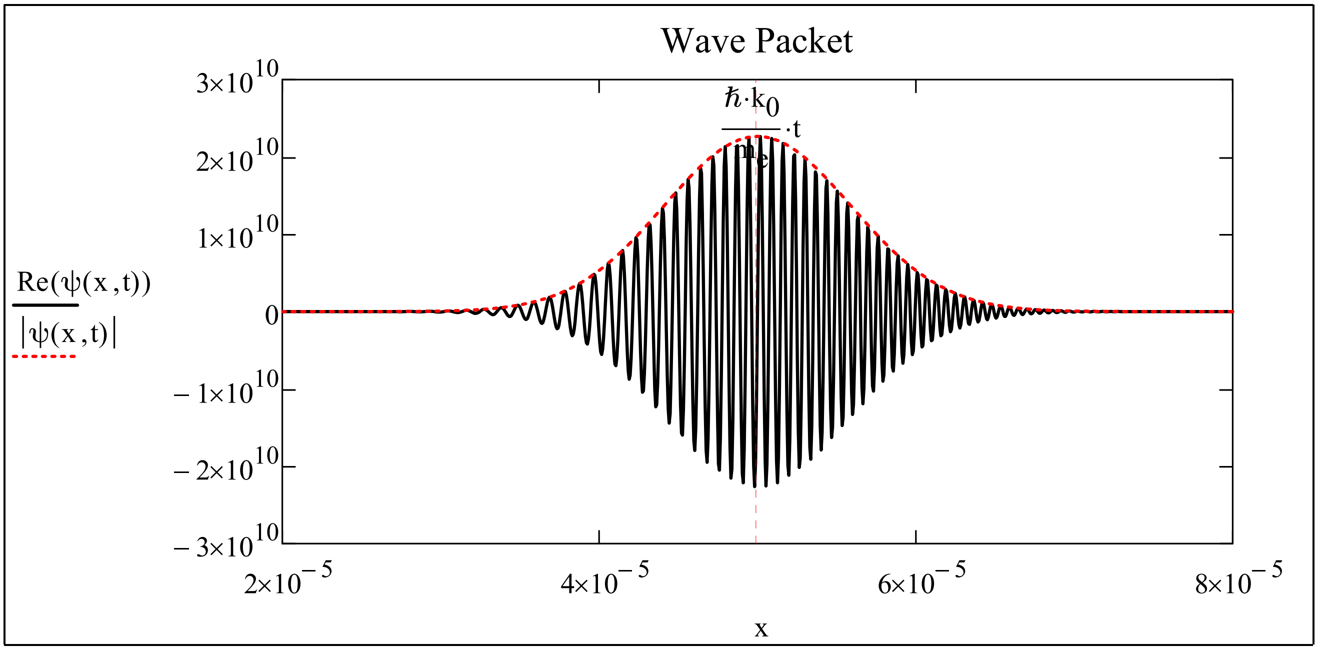
$$A := \frac{1}{\sqrt{a\cdot\sqrt{\pi}}} \qquad k_0 := \frac{m_e\cdot v}{\hbar} \qquad v_0 := \frac{\hbar}{m_e}\cdot k_0 \qquad p_0 := \hbar\cdot k_0$$

$$A = 751.126\,\frac{1}{m^{0.5}} \qquad k_0 = 8.637\times 10^{6}\,\frac{1}{m}$$

$$\psi(x,t) := \frac{A}{\sqrt{1+\frac{i\cdot\hbar\cdot t}{m_e\cdot a^2}}}\cdot\exp\left[\frac{-\left(x^2-2\cdot i\cdot a^2\cdot k_0\cdot x+\frac{i\cdot\hbar\cdot t}{2\cdot m_e}\cdot k_0^{\,2}\cdot a^2\right)}{2\cdot a^2\cdot\left(1+\frac{i\cdot\hbar\cdot t}{m_e\cdot a^2}\right)}\right]$$

$a = 1\cdot\mu m \qquad v = 1\times10^{3}\,\frac{m}{s} \qquad t := 50\cdot ns$

$$x := 10^{-5}\cdot2\cdot m,\, 10^{-5}\cdot2\cdot m + \frac{10^{-5}\cdot8\cdot m - 10^{-5}\cdot2\cdot m}{1000} \,..\, 10^{-5}\cdot8\cdot m$$



$$\psi\left(10^{-5}\cdot5\cdot m, t\right) = \left(-4.568\times10^{5} - 2.265j\times10^{10}\right)\frac{1}{m^{0.5}}$$

$$\xi = \frac{k}{k_0}$$

$$C0(\xi) := \frac{A\cdot a}{\sqrt{2\cdot\pi}}\cdot\exp\left[\frac{-1}{2}\cdot a^{2}\cdot k_0^{\,2}\cdot(\xi-1)^{2}\right]$$

$$v_{ph}(\omega, k) := \frac{\omega(k)}{k}$$

$$p_0 = 0\,\frac{m\cdot kg}{s}$$

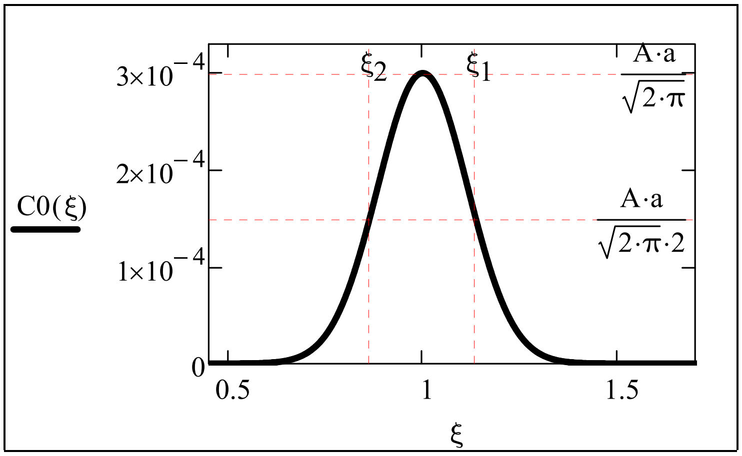
$$k_0 = 8.637\times10^{6}\,\frac{1}{m}$$

$$v_{ph}\left(\omega, k_0\cdot\frac{3}{2}\right) = 750\,\frac{m}{s}$$

Abscissa of the widths at half height:

$$\xi_1 := \sqrt{\frac{\ln\left(\frac{1}{2}\right)}{\left(\frac{-1}{2}\cdot a^{2}\cdot k_0^{\,2}\right)}} + 1 \qquad \xi_2 := -\sqrt{\frac{\ln\left(\frac{1}{2}\right)}{\left(\frac{-1}{2}\cdot a^{2}\cdot k_0^{\,2}\right)}} + 1 \qquad \xi_1 - \xi_2 = 0.273$$

$$\xi := 0.4, .4 + .001 .. 2.2$$

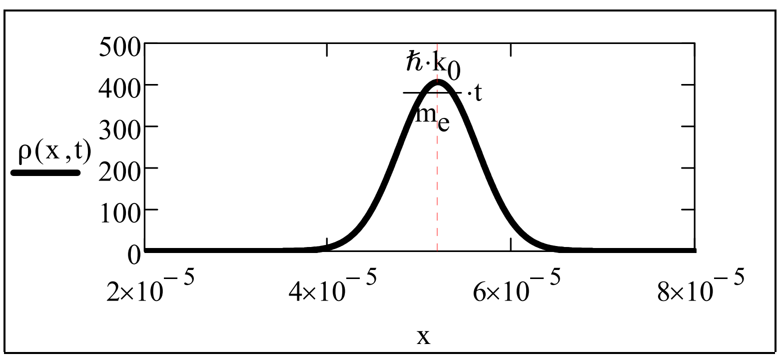


A good understanding of (16.55) which is asomewhat complicated expression, can be obtained by debating the density a flow again. The first one becomes:

$$\rho(x,t) := \frac{(|A|)^2}{\left[1 + \left(\frac{\hbar \cdot t}{m_e \cdot a^2}\right)^2\right]^2} \cdot \exp\left[\frac{-\left(x - \frac{\hbar \cdot k_0}{m_e} \cdot t\right)^2}{a^2 \cdot \left[1 + \left(\frac{\hbar \cdot t}{m_e \cdot a^2}\right)^2\right]}\right] \qquad (16.56)$$

which is a function of x, it is a bell curve, whose maximum is shifted from x=0 to x=($\hbar k_0$/m)t.

$$t := 10^{-9} \cdot 52 \cdot s$$



The maximum of the "wave group" represented by (16.55) is thus propagated at a velocity $v_0 = \hbar k / m$ ('group velocity = particle velocity'). the denominator of the exponent in (16.56) shows that, at the same time, the wave packet has expand from its initial width - a - at the instant t = 0, to

$$v_0 := \frac{\hbar \cdot k_0}{m_e} \qquad a_1 := a \cdot \sqrt{\left[1 + \left(\frac{\hbar \cdot t}{m_e \cdot a^2}\right)^2\right]} \qquad a_1 = 6.103 \times 10^{-6} m$$

$$v_0 = 1 \times 10^3 \frac{m}{s} \qquad a = 1 \times 10^{-6} m$$

Which is about equal to $\hbar t$ / (ma) at the instant t = t. This effect can be easily explained by the spectral function C (k): t waveform spectrum has the width **Δ**k = 1 / a, the partial wave velocities cover a region of width

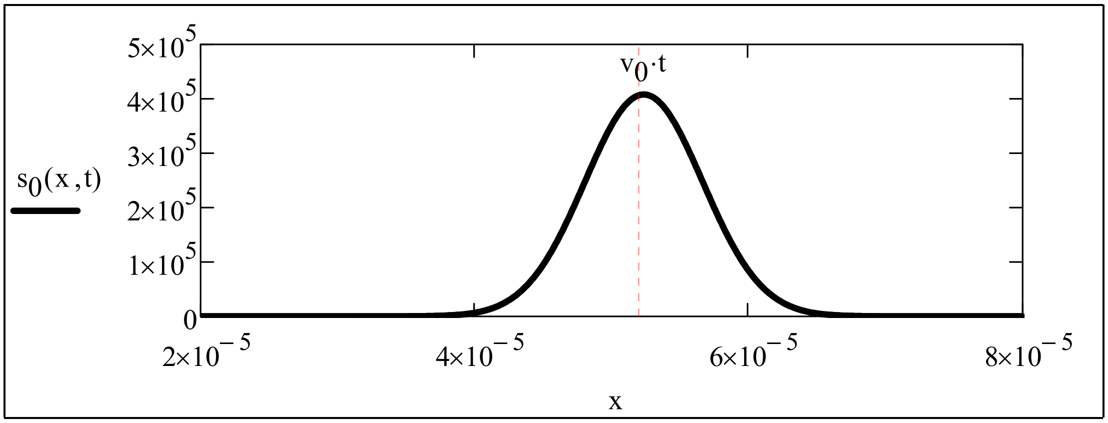
$$\Delta v = (\hbar / k)\, \Delta k = \hbar / (ma)$$

so that the packet widens to **Δ**x = t**Δ**v = $\hbar t$ / (ma). The flow is derived from (16.55) with the help of the relationship:

$$\frac{\partial}{\partial x}\psi(x,t) = i\cdot k_0\cdot\frac{\left(1+i\cdot\frac{x}{a^2\cdot k_0}\right)}{1+i\cdot\frac{\hbar\cdot t}{m\cdot a^2}}\cdot\psi(x,t)$$

Which compared with (16.55) provides:

$$s_0(x,t) := \rho(x,t)\cdot v_0\cdot\frac{1+\frac{\hbar\cdot t\cdot x}{m_e\cdot a^4\cdot k_0}}{1+\left(\frac{\hbar\cdot t}{m_e\cdot a^2}\right)^2} \qquad (16.57)$$



It follows that in no way I always have $s = rv_0$ at every instant, as I have for $t = 0$.
This is again a consequence of the finite width of the spectrum: at the maximum point of the packet, $x_0 = v_0 t$, the equati (16.57) leads to the elementary relation $s = \rho v_0$ for $x < x_0$ or $x > x_0$ I find $s < \rho v_0$, $s > \rho v_0$ this is reasonable as at a point x ($x > x_0$) must reach those parts of the wave packet whose speeds are lower (higher) than v_0. Finally, I can mention that tl normalization condition always applies at any instant, this reflects the conservation of matter.

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

Standing wave

Infinitely heigh potential barrier

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

Classical Hamiltonian for two non relativistic particles of rest mass m1 and m2 , under mutual interaction only

Classical Hamiltonian for two non relativistic and non interacting particles of rest mass m1 and m2

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 Δ From Each Other

17 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	
$\mathbf{p}$	$\leftrightarrow -i\cdot\hbar\cdot\nabla$	(17.1)
$\mathbf{L} = \mathbf{r}\times\mathbf{p}$	$\leftrightarrow -i\cdot\hbar\cdot\mathbf{r}\times\nabla,$	(17.2)
$\mathbf{s}\cdot\mathbf{p}$	$\leftrightarrow \nabla\times$ A. M. 551	
$\mathbf{p}^2$	$\leftrightarrow -\hbar^2\cdot\Delta,$	(17.3)
$\frac{\mathbf{p}\cdot\mathbf{q'}}{2} = \frac{\mathbf{p}^2}{2\cdot m}$	$\leftrightarrow \frac{-\hbar^2}{2\cdot m}\cdot\Delta$	(17.4)
Energy E	$\leftrightarrow i\cdot\hbar\cdot\frac{\partial}{\partial t},$	(17.5)
E^2	$\leftrightarrow -\hbar\cdot\frac{\partial^2}{\partial t^2}$	
$\ell^2 = (\mathbf{r}\times\mathbf{p})\cdot(\mathbf{r}\times\mathbf{p}) = r^2\cdot\left(\mathbf{p}^2 - p_r^{\,2}\right)$	$\leftrightarrow r^2\cdot\left[-\hbar^2\cdot\Delta + \hbar^2\cdot\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\right]$ Sph. coord.	(17.6)
$\mathbf{r}\cdot\mathbf{p}$	$\leftrightarrow -i\cdot\hbar\cdot r\cdot\frac{\partial}{\partial r} = -i\cdot\hbar\cdot r\cdot\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$ Sph. coord.	(17.7)
$\mathbf{A}$ is the vector potential $\mathbf{p}\cdot\mathbf{A}$	$\leftrightarrow \frac{i\cdot\hbar}{2}\cdot(\nabla\bullet\mathbf{A} + \mathbf{A}\cdot\nabla).$	(17.8)

Example 17.1) *Heisenberg Uncertainty principle* $\boxed{\Delta\,\mathbf{A}\cdot\Delta\,\mathbf{B} \ge \frac{1}{2}\cdot\left|<[\,\mathbf{A},\mathbf{B}\,]>\right|}$

For a particle of mass m

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

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

$$[\,x,p\,] = i\cdot\hbar$$

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

$$\Delta\,x\cdot\Delta\,p \ge \frac{1}{2}\cdot\hbar$$

$$x = \mathbf{q} \qquad \mathbf{q} \leftrightarrow \mathbf{q} = \mathbf{A} \qquad \mathbf{p} = \hbar\cdot\mathbf{k} = \hbar\cdot\frac{2\cdot\pi}{\lambda}\cdot\mathbf{k} = \hbar\cdot\frac{\omega}{c}\cdot\mathbf{k} = \frac{E}{c}\cdot\mathbf{k} \qquad \mathbf{p} \leftrightarrow \left(\frac{\hbar}{i}\cdot\nabla = \mathbf{B}\right)$$

$$\frac{\Delta x}{c} = \Delta t \qquad \Delta\,x\cdot\frac{1}{c}\cdot\Delta\,E = \Delta t\cdot\Delta E \ge \frac{1}{2}\cdot\hbar$$

Example 17.2) The Hamiltonian **H** and the operator **A,** are time independent.

$$\mathbf{A} = x \quad \mathbf{p} \leftrightarrow \left(\frac{\hbar}{i}\cdot\nabla\right) \qquad \mathbf{H} = \mathbf{T} + \mathbf{U} = \frac{\mathbf{p}^2}{2\cdot m} = -\frac{\hbar^2}{2\cdot m}\cdot\nabla^2$$

$$\left(\left[x, -\frac{\hbar^2}{2\cdot m}\cdot\nabla^2 \right]\right)\psi = -x\cdot\frac{\hbar^2}{2\cdot m}\cdot\nabla^2\,\psi + \frac{\hbar^2}{2\cdot m}\cdot\nabla^2\,\psi\cdot x = 0$$

$$\Delta\, x\cdot\Delta\left(-\frac{\hbar^2}{2\cdot m}\cdot\nabla^2\right) \geq \frac{1}{2}\cdot\left| < \left[x, -\frac{\hbar^2}{2\cdot m}\cdot\nabla^2 \right] > \right| = 0$$

Example 17.3) Relativistic case: $E = \pm\, c\cdot\sqrt{p^2 + m^2\cdot c^2}$

$$E^2 = c^2\cdot p^2 + m^2\cdot c^4$$

$$-\hbar^2\cdot\frac{\partial^2}{\partial t^2}\Psi = -c^2\cdot\hbar^2\cdot\Delta\Psi + m^2\cdot c^4\cdot\Psi$$

$$\Delta\Psi - \frac{1}{c^2}\cdot\frac{\partial^2}{\partial t^2}\Psi - \frac{m^2\cdot c^2}{\hbar^2}\cdot\Psi = 0$$

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

Klein-Gordon equation: $\left[\square + \left(\frac{m\cdot c}{\hbar}\right)^2\right]\Psi(\mathbf{r}, t) = 0$

18 Lagrange equations

Lagrangian coordinates for a system with n degree of freedom : $\mathbf{q}_i$, i=1,..n

Kinetic energy : T
Potential energy : U

Classical mechanics Lagrangian :

$$\mathcal{L}(q_1, q_2, ...q_n, q'_1, q'_{2.n}, ...q', t) = \mathbf{T}(q'_1, q'_2, ...q'_n, t) - \mathbf{U}(q_1, q_2, ...q_n) \tag{18.1}$$

Lagrange equations' system $\frac{d}{dt}\frac{\partial}{\partial \mathbf{q'_i}}\mathcal{L}_i(q_1, q_2, ...) - \frac{\partial}{\partial \mathbf{q}_i}\mathcal{L}_i(q_1, q_2, ...) = 0 \quad i = 1, 2, 3 .. n$ (18.2)

Conjugated momenta $\mathbf{p_i} = \frac{\partial}{\partial \mathbf{q'_i}}\mathcal{L} \qquad i = 1, 2, 3 .. n$ Kinetic energy: $T = \frac{1}{2 \cdot m} \cdot \sum_{i=1}^{n} \mathbf{p_i}^2 = \frac{1}{2 \cdot m} \cdot \sum_{i=1}^{n} \left(\frac{\partial}{\partial \mathbf{q'_i}}\mathcal{L}\right)^2$

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

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

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

19 Hamilton equations

Kinetic energy : T, Potential energy : U

Classical mechanics Hamiltonian :

$$\mathcal{H}(q_1, q_2, ...q_n, p_1, p_2, ...p_n, t) = T + U = 2 \cdot T - \mathcal{L}(q_1, q_2, ...q_n, q'_1, q'_{2.n}, ...q', t) = E$$

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

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

$$\boxed{\mathbf{q'}_i = \frac{\partial}{\partial \mathbf{p}_i}\mathcal{H}} \qquad i = 1, 2, 3 .. n \tag{19.2}$$

$$\boxed{\mathbf{p'}_i = -\frac{\partial}{\partial \mathbf{q}_i}\mathcal{H}} \qquad \text{19.3)}$$

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:

$$i\cdot\hbar\cdot\frac{\partial}{\partial t}|\psi> = \mathbf{H}|\psi> \tag{20.1}$$

$$-i\cdot\hbar\cdot\frac{\partial}{\partial t}<\psi| = <\psi|\mathbf{H}^{\dagger} \tag{20.2}$$

They are deterministic.

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

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

$$\mathbf{H}|k> = E_k|k>, \tag{20.3}$$

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

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

$$\mathbf{P_n} = \sum_{k=1}^{N}|k><k| = 1 \tag{20.5}$$

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

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

$$i\cdot\hbar\cdot\sum_{k=1}^{N}|k>\frac{\partial}{\partial t}<k|\psi> = \sum_{k=1}^{N}|k><k|\mathbf{H}|\psi> \tag{20.7}$$

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

$$i\cdot\hbar\cdot\sum_{k=1}^{N}|k>\frac{\partial}{\partial t}<k|\psi> = \sum_{k=1}^{N}|k><k|E_k|\psi> \tag{20.8}$$

$$i\cdot\hbar\cdot\sum_{k=1}^{N}|k>\frac{\partial}{\partial t}<k|\psi> - \sum_{k=1}^{N}|k><k|E_k|\psi> = 0 \tag{20.9}$$

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

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

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

$$i\cdot\hbar\cdot\frac{\partial}{\partial t}<k\,|\,\psi> - E_k<k\,|\,\psi> = 0 \tag{20.12}$$

the solution is: $$<k\,|\,\psi> = C\cdot e^{-i\cdot\frac{E_k}{\hbar}\cdot t} \tag{20.13}$$

and the initial condition let me know the constant C:

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

$$|\,k><k\,|\,\psi> = |\,k><k\,|\,\psi_0> e^{-i\cdot\frac{E_k}{\hbar}\cdot(t-t_0)} \tag{20.15}$$

$$|\,k><k\,| = 1 \qquad |\,\psi> = |\,\psi_0> e^{-i\cdot\frac{E_k}{\hbar}\cdot(t-t_0)} \tag{20.16}$$

$$f(\mathbf{H})\,|\,k> = f(E_k)\,|\,k> \tag{20.17}$$

$$f(\mathbf{H}) = \sum_{k=1}^{N} |\,k> f(E_k) <k\,| = \sum_{k=1}^{N} |\,k> e^{-i\cdot\frac{E_k}{\hbar}\cdot(t-t_0)} <k\,| = \sum_{k=1}^{N} |\,k> e^{-i\cdot\frac{\mathbf{H}}{\hbar}\cdot(t-t_0)} <k\,| \tag{20.18}$$

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

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

$$\frac{E_k}{\hbar} = \omega_k \tag{20.20}$$

Einstein equation $$E(\omega_k) := \hbar\cdot\omega_k \tag{20.21}$$

Time evolution operator

Time evolution operator (conservative system, the Hamiltonian **H,** is constant in time):

$$\boxed{\mathbf{U}(t,t_0) = e^{-i\cdot\frac{\mathbf{H}\cdot(t-t_0)}{\hbar}}} \qquad \mathbf{U}(t_0,t_0) = 1 \tag{20.22}$$

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

If **H** is time independent then: $\boxed{i\cdot\hbar\cdot\frac{d}{dt}\mathbf{U}(t,t_0) = \mathbf{H}\cdot\mathbf{U}(t,t_0)}$ (20.23)

Integral equation $\boxed{\mathbf{U}(t,t_0) = 1 - \frac{i}{\hbar}\cdot\int_{t_0}^{t}\mathbf{H}\cdot\mathbf{U}(\tau,t_0)\,d\tau}$ (20.24)

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

$$\boxed{|\ \Psi(t) > = \mathbf{U}(t,t_0)\ |\ \Psi(t_0) >} \qquad (20.25)$$

Differentiation: $\frac{d}{dt}|\ \Psi(t) > = \left(\frac{d}{dt}\mathbf{U}(t,t_0)\right)|\ \Psi(t_0) >$ (20.26)

from (20.19) 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 (20.22) gives:

$$\frac{d}{dt}|\ \Psi(t) > = \frac{-i}{\hbar}\cdot\mathbf{H}\cdot\mathbf{U}(t,t_0)\ |\ \Psi(t_0) > \qquad (20.27)$$

that is the ***Schrödinger equation:*** $\boxed{\frac{d}{dt}|\ \Psi(t) > = \frac{-i}{\hbar}\cdot\mathbf{H}\ |\ \Psi(t) >}$ (20.28)

Time evolution operator

21 *Momentum Space Wave Function*

$dV = dx\cdot dy\cdot dz \qquad d\,\mathbf{k} = d\,k_x\cdot d\,k_y\cdot d\,k_z \qquad \mathbf{k} = k_x\cdot\mathbf{i_x} + k_y\cdot\mathbf{i_y} + k_z\cdot\mathbf{i_z}$

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

$$\boxed{\Psi(\mathbf{r}) = \frac{1}{\sqrt{(2\cdot\pi)^3}}\cdot\int f(\mathbf{k})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k}} \qquad \boxed{f(\mathbf{k}) = \frac{1}{\sqrt{(2\cdot\pi)^3}}\cdot\int \Psi(\mathbf{r})\cdot e^{-i\cdot\mathbf{k}\cdot\mathbf{r}}\,dV} \qquad (21.1)$$

$$\boxed{V(\mathbf{r}) = \int W(\mathbf{k})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k}} \qquad \lim_{r\to\infty} V(\mathbf{r}) = 0 \qquad \boxed{W(\mathbf{k}) = \frac{1}{(2\cdot\pi)^3}\cdot\int V(\mathbf{r})\cdot e^{-i\cdot\mathbf{k}\cdot\mathbf{r}}\,dV} \qquad (21.2)$$

Substitute into the Schrödinger equatio $\frac{-\hbar^2}{2\cdot m}\cdot\Delta\ \Psi(r) + V(r)\ \Psi(r) = E\ \Psi(r)$ (21.3)

Calculation of the MOMENTUM SPACE WAVE FUNCTION [3]

$$\left[\frac{-\hbar^2}{2\cdot m}\cdot\frac{1}{\sqrt{(2\cdot\pi)^3}}\cdot\Delta\int f(\mathbf{k})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k}\ ...\ + \frac{1}{\sqrt{(2\cdot\pi)^3}}\cdot\int W(\mathbf{k})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k}\cdot\int f(\mathbf{k_1})\cdot e^{i\cdot\mathbf{k_1}\cdot\mathbf{r}}\,d\mathbf{k_1}\right] = E\cdot\frac{1}{\sqrt{(2\cdot\pi)^3}}\int f(\mathbf{k})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k} \tag{21.4'}$$

$$\frac{-\hbar^2}{2\cdot m}\cdot\int f(\mathbf{k})\cdot\Delta\, e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k} + \int W(\mathbf{k})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k}\cdot\int f(\mathbf{k_1})\cdot e^{i\cdot\mathbf{k_1}\cdot\mathbf{r}}\,d\mathbf{k_1} = E\cdot\int f(\mathbf{k})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k} \tag{21.5'}$$

consider the the second term on the left side:

$$\int W(\mathbf{k})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k}\int f(\mathbf{k_1})\cdot e^{i\cdot\mathbf{k_1}\cdot\mathbf{r}}\,d\mathbf{k_1} = \int\int W(\mathbf{k})\cdot f(\mathbf{k_1})\cdot e^{i\cdot(\mathbf{k_1}+\mathbf{k})\cdot\mathbf{r}}\,d\mathbf{k}\,d\mathbf{k_1} \tag{21.6'}$$

replace $\mathbf{k_2} = \mathbf{k}+\mathbf{k_1}$ $\quad \mathbf{k_1} = \mathbf{k_2}-\mathbf{k}$ $\quad d\,\mathbf{k_1} = d\,\mathbf{k_2}$ $\quad \mathbf{k} = \mathbf{k_2}-\mathbf{k_1}$ $\quad d\,\mathbf{k} = d\,\mathbf{k_2}$ (21.7')

obtaining
$$\int\int W(\mathbf{k})\cdot f(\mathbf{k_1})\cdot e^{i\cdot(\mathbf{k_1}+\mathbf{k})\cdot\mathbf{r}}\,d\mathbf{k}\,d\mathbf{k_1} = \int\int W(\mathbf{k_2}-\mathbf{k_1})\cdot f(\mathbf{k_1})\cdot e^{i\cdot\mathbf{k_2}\cdot\mathbf{r}}\,d\mathbf{k_1}\,d\mathbf{k_2} \tag{21.8'}$$

$$\mathbf{k_2} = \mathbf{k} \tag{21.9'}$$

resulting
$$\int\int W(\mathbf{k_2}-\mathbf{k_1})\cdot f(\mathbf{k_1})\cdot e^{i\cdot\mathbf{k_2}\cdot\mathbf{r}}\,d\mathbf{k_1}\,d\mathbf{k_2} = \int\int W(\mathbf{k}-\mathbf{k_1})\cdot f(\mathbf{k_1})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k_1}\,d\mathbf{k} \tag{21.10'}$$

furthermore $\Delta\, e^{i\cdot\mathbf{k}\cdot\mathbf{r}} = -\mathbf{k}^2\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}$ (21.11')

$$\frac{\hbar^2}{2\cdot m}\cdot\int f(\mathbf{k})\cdot\mathbf{k}^2\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k} + \int\int W(\mathbf{k}-\mathbf{k_1})\cdot f(\mathbf{k_1})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k_1}\,d\mathbf{k} = E\cdot\int f(\mathbf{k})\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k} \tag{21.12'}$$

$$\int\left[\left(\frac{\hbar^2}{2\cdot m}\cdot\mathbf{k}^2 - E\right)\cdot f(\mathbf{k}) + \int W(\mathbf{k}-\mathbf{k_1})\cdot f(\mathbf{k_1})\,d\mathbf{k_1}\right]\cdot e^{i\cdot\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k} = 0 \tag{21.13'}$$

$$\left(\frac{\hbar^2}{2\cdot m}\cdot\mathbf{k}^2 - E\right)\cdot f(\mathbf{k}) + \int W(\mathbf{k}-\mathbf{k_1})\cdot f(\mathbf{k_1})\,d\mathbf{k_1} = 0 \tag{21.14'}$$

Calculation of the MOMENTUM SPACE WAVE FUNCTION [3]

integral equation
$$\boxed{\int W(\mathbf{k}-\mathbf{k_1})\cdot f(\mathbf{k_1})\,d\mathbf{k_1} = -\left(\frac{\hbar^2}{2\cdot m}\cdot\mathbf{k}^2 - E\right)\cdot f(\mathbf{k})} \tag{21.4}$$

22 Representations theory

Euclidean representation: $< x \mid \Psi > = \Psi(x), \quad < \Psi \mid x > = \Psi(x)^*,$

k representation: $< k \mid \Psi > = \Psi(k), \quad < \Psi \mid k > = \Psi(k)^*,$

p representation: $< p \mid \Psi > = \Psi(p), \quad < \Psi \mid p > = \Psi(p)^*,$

Closure relation: $$\mathbf{P_A} = \sum_{j=1}^{N} \mid j >< j \mid + \int_{\xi_1}^{\xi_2} \mid \xi > d\xi < \xi \mid = 1 \qquad (10.12')$$

$$\mathbf{P_A}\,\mathbf{H} = \sum_{j=1}^{N} \mid j >< j \mid \mathbf{H} + \int_{\xi_1}^{\xi_2} \mid \xi > d\xi < \xi \mid \mathbf{H} = \sum_{j=1}^{N} \frac{\mid j >< j \mid}{\lambda_j} + \frac{\int_{\xi_1}^{\xi_2} \mid \xi > d\xi < \xi \mid}{\lambda}$$

$$\mathbf{P_A} = \sum_{j=1}^{N} \mid j >< j \mid = 1$$

$$\mathbf{H} \mid \psi > = E_k \mid \psi >$$

$$(z - \mathbf{H}) \mid \psi > = (z - E_k) \mid \psi >$$

$$(z - \mathbf{H}) \cdot \mathbf{P_A} \mid \psi > = (z - E_k) \cdot \mathbf{P_A} \mid \psi >$$

apply the closure relation (10.12') assuming that there is no continuous spectrum

$$(z - \mathbf{H}) \cdot \sum_{j=1}^{N} \mid j >< j \mid \psi > = (z - E_k) \cdot \sum_{j=1}^{N} \mid j >< j \mid \psi >$$

$$(z - \mathbf{H})^{-1} \cdot \sum_{j=1}^{N} \mid j >< j \mid \psi > = \frac{1}{(z - E_k)} \cdot \sum_{j=1}^{N} \mid j >< j \mid \psi >$$

$$(z - \mathbf{H})^{-1} \cdot \sum_{j=1}^{N} \mid j >< j \mid = \frac{1}{(z - E_k)} \cdot \sum_{j=1}^{N} \mid j >< j \mid = \sum_{j=1}^{N} \frac{\mid j >< j \mid}{z - E_k} = G(z)$$

Green function: $$G(z) = \sum_{j=1}^{N} \frac{\mid j >< j \mid}{z - E_k}$$

23 Time evolution of the average value of an observable [4]

$$\frac{d}{dt} < \mathbf{A} > = \frac{1}{i \cdot \hbar} \cdot \left(< [\, \mathbf{A}, \mathbf{H} \,] > \right) + < \frac{\partial}{\partial t} \mathbf{A} > \qquad (23.1)$$

Demonstration of 23.1)

Consider the definition of average value:

$$< \mathbf{A} > = < \psi \mid \mathbf{A} \mid \psi > = \int \Psi(\tau)^* \cdot \mathbf{A} \cdot \Psi(\tau)\, d\tau \tag{23.2}$$

and calculate the expectation value derivative:

$$\frac{d}{dt} < \mathbf{A} > = \frac{d}{dt} < \psi \mid \mathbf{A} \mid \psi > \tag{23.3}$$

$$\text{calculation result: } \frac{d}{dt} < \mathbf{A} > = \left(\frac{\partial}{\partial t} < \psi \mid \right) \mathbf{A} \mid \psi > + < \psi \mid \frac{\partial}{\partial t} \mathbf{A} \mid \psi > + < \psi \mid \mathbf{A} \frac{\partial}{\partial t} \mid \psi > \tag{23.4}$$

$$\text{knowing that: } i \cdot \hbar \cdot \frac{\partial}{\partial t} \mid \psi > = \mathbf{H} \mid \psi > \quad \text{and} \quad -i \cdot \hbar \cdot \frac{\partial}{\partial t} < \psi \mid = < \psi \mid \mathbf{H}^\dagger \tag{23.5}$$

$$\text{from which } \frac{\partial}{\partial t} \mid \psi > = \frac{1}{i \cdot \hbar} \cdot \mathbf{H} \mid \psi > \quad \text{and} \quad \frac{\partial}{\partial t} < \psi \mid = < \psi \mid \mathbf{H}^\dagger \cdot \frac{1}{-i \cdot \hbar} \tag{23.6}$$

$$< \psi \mid \frac{\partial}{\partial t} \mathbf{A} \mid \psi > = < \frac{\partial}{\partial t} \mathbf{A} >$$

after a substitution in 22.4), I get

$$\frac{d}{dt} < \mathbf{A} > = \left(\frac{\partial}{\partial t} < \psi \mid \right) \mathbf{A} \left(\mid \psi >\right) + < \psi \mid \mathbf{A} \frac{\partial}{\partial t} \mid \psi > \ldots = \left(< \psi \mid \mathbf{H}^\dagger \cdot \frac{1}{-i \cdot \hbar}\right) \mathbf{A} \left(\mid \psi >\right) \ldots$$

$$+ < \frac{\partial}{\partial t} \mathbf{A} > \qquad + < \psi \mid \mathbf{A} \left(\frac{1}{i \cdot \hbar} \cdot \mathbf{H} \mid \psi >\right) + < \frac{\partial}{\partial t} \mathbf{A} >$$

$$\text{so that} \quad \frac{d}{dt} < \mathbf{A} > = \left(< \psi \mid \mathbf{H}^\dagger \cdot \frac{1}{-i \cdot \hbar}\right) \mathbf{A} \left(\mid \psi >\right) + < \psi \mid \mathbf{A} \left(\frac{1}{i \cdot \hbar} \cdot \mathbf{H} \mid \psi >\right) + < \frac{\partial}{\partial t} \mathbf{A} >$$

$$\frac{d}{dt} < \mathbf{A} > = -\frac{1}{i \cdot \hbar} \left(< \psi \mid \mathbf{H}^\dagger \cdot \mathbf{A} \mid \psi >\right) + \frac{1}{i \cdot \hbar} \left(< \psi \mid \mathbf{H} \cdot \mathbf{A} \mid \psi >\right) + < \frac{\partial}{\partial t} \mathbf{A} >$$

$$\text{namely} \quad \frac{d}{dt} < \mathbf{A} > = \frac{1}{i \cdot \hbar} \cdot \left(< \psi \mid \mathbf{A} \cdot \mathbf{H} \mid \psi > - < \psi \mid \mathbf{H}^\dagger \cdot \mathbf{A} \mid \psi >\right) + < \frac{\partial}{\partial t} \mathbf{A} > \tag{23.7}$$

Self adjoint Operator (Hermitian): $\mathbf{H} = \mathbf{H}^\dagger$

$$\frac{d}{dt} < \mathbf{A} > = \frac{1}{i \cdot \hbar} \cdot < \psi \mid (\mathbf{A} \cdot \mathbf{H} - \mathbf{H} \cdot \mathbf{A}) \mid \psi > + < \frac{\partial}{\partial t} \mathbf{A} > \tag{23.8}$$

$$\frac{d}{dt} < \mathbf{A} > = \frac{1}{i \cdot \hbar} \cdot \left(< [\, \mathbf{A}, \mathbf{H} \,] >\right) + < \frac{\partial}{\partial t} \mathbf{A} >$$

Demonstration of 23.1)

$$\frac{d^2}{dt^2} < \mathbf{A} > = -\frac{1}{\hbar^2} < [\, [\, \mathbf{A}, \mathbf{H} \,], \mathbf{H} \,] > + \frac{1}{i \cdot \hbar} < \frac{d}{dt} [\, \mathbf{A}, \mathbf{H} \,] > + \frac{\partial}{\partial t} < \frac{\partial}{\partial t} \mathbf{A} > \tag{23.9}$$

Demonstration of 23.9)

Eq. 23.1 can be rewritten as: $< \frac{\partial}{\partial t}\mathbf{A} > = -\frac{1}{i\cdot\hbar} < [\,\mathbf{A},\mathbf{H}\,] > + \frac{d}{dt} < \mathbf{A} >$ (23.10)

For a system in stationary state, of energy $E(\omega) := \hbar\cdot\omega$ $\quad | \Psi > = e^{-i\cdot\frac{E\cdot t}{\hbar}} | \psi >$

$$E\cdot\psi\cdot e^{-\frac{E\cdot t\cdot i}{\hbar}} = \mathbf{H}\left(\psi\cdot e^{-i\cdot\frac{E\cdot t}{\hbar}}\right)$$

Schrödinger equation for the stationary state $\mathbf{H}\cdot\psi = E\cdot\psi$ $\qquad \mathbf{H} \,|\, \psi_k > = E_k \,|\, \psi_k >$

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.

24 Conservation Laws [4]

For a particle in a scalar potential:

Probability density $$P = \psi^{*}\cdot\psi \tag{24.1}$$

Probability current density $$\mathbf{J} = \frac{\hbar}{2\cdot m\cdot i}\cdot\left[\psi^{*}\cdot\nabla\psi - (\nabla\psi)^{*}\psi\right] \tag{24.2}$$

Continuity law $$\nabla\cdot\mathbf{J} + \frac{\partial}{\partial t}P = 0 \tag{24.3}$$

Energy Flux vector $$\mathbf{S} = -\frac{\hbar^2}{2\cdot m}\cdot\left[\frac{\partial}{\partial t}\psi^{*}\cdot\nabla\psi - \frac{\partial}{\partial t}\psi\cdot\nabla(\psi^{*})\right] \tag{24.4}$$

Energy density $$W = \frac{\hbar^2}{2\cdot m}\cdot\left[\nabla(\psi^{*})\cdot\nabla\psi + \psi^{*}\cdot\nabla\psi\right] \tag{24.5}$$

25 Commutation relations of Angular Momentum [4]

(Classical mechanics $\mathbf{L} = \mathbf{r} \times \mathbf{p}$)

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \leftrightarrow -i\cdot\hbar\cdot\mathbf{r} \times \nabla, \tag{25.1}$$

$$[\ \mathbf{q_i}, \mathbf{A}(\mathbf{p_i}, \mathbf{q_i})\ ] = -i\cdot\hbar\cdot\frac{\partial}{\partial \mathbf{q_i}}\mathbf{A}(\mathbf{p_i}, \mathbf{q_i}) \tag{25.2}$$

$$[\ \mathbf{L_x}, \mathbf{L_y}\ ] = i\cdot\hbar\cdot\mathbf{L_z} \tag{25.3}$$

$$[\ \mathbf{L_y}, \mathbf{L_z}\ ] = i\cdot\hbar\cdot\mathbf{L_x} \tag{25.4}$$

$$[\ \mathbf{L_z}, \mathbf{L_x}\ ] = i\cdot\hbar\cdot\mathbf{L_y} \tag{25.5}$$

$$[\ \mathbf{L_z}, \mathbf{L_x}^2\ ] = i\cdot\hbar\cdot(\mathbf{L_y}\cdot\mathbf{L_x} + \mathbf{L_x}\cdot\mathbf{L_y}) \tag{25.6}$$

$$[\ \mathbf{L_z}, \mathbf{L_y}^2\ ] = i\cdot\hbar\cdot(\mathbf{L_y}\cdot\mathbf{L_x} + \mathbf{L_x}\cdot\mathbf{L_y}) \tag{25.7}$$

$$[\ \mathbf{L_z}, \mathbf{L_z}^2\ ] = 0 \tag{25.8}$$

u is a unit vector $[\ \mathbf{u}\cdot\mathbf{L}, \mathbf{p}\ ] = -i\cdot\hbar\cdot(\mathbf{i_x} \times \mathbf{p})$ (25.9)

u is a unit vector $[\ \mathbf{u}\cdot\mathbf{L}, \mathbf{r}\ ] = -i\cdot\hbar\cdot(\mathbf{i_x} \times \mathbf{r})$ (25.10)

u is a unit vector $[\ \mathbf{u}\cdot\mathbf{L}, \mathbf{p}^2\ ] = 0$ (25.11)

u is a unit vector $[\ \mathbf{u}\cdot\mathbf{L}, r^2\ ] = 0$ (25.12)

u is a unit vector $[\ \mathbf{u}\cdot\mathbf{L}, \mathbf{r}\cdot\mathbf{p}\ ] = 0$ (25.13)

Spherical coordinates (r,θ,φ) $\quad p_r = \frac{\hbar}{i}\cdot\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$ (25.14)

Classical mechanics $\quad \mathbf{p}^2 = \mathbf{p_r}^2 + \frac{\mathbf{L}^2}{r^2}$ (25.15)

$$\mathbf{L}^2 = \frac{\hbar^2}{\sin(\theta)^2}\cdot\left[\sin(\theta)\cdot\left[\frac{\partial}{\partial\theta}\left(\sin(\theta)\cdot\frac{\partial}{\partial\theta}\right)\right] + \frac{\partial^2}{\partial\varphi^2}\right] \tag{25.16}$$

$$\mathbf{L}^2\,Y(\ell, m, \theta, \varphi) = \ell\cdot(\ell + 1)\cdot\hbar^2\cdot Y(\ell, m, \theta, \varphi) \qquad \ell = 0, 1, 2, \ldots, \infty \tag{25.17}$$

$$\mathbf{L_z}\,Y(\ell, m, \theta, \varphi) = m\cdot\hbar\cdot Y(\ell, m, \theta, \varphi) \qquad m = -\ell, -\ell + 1, \ldots, \ell \tag{25.18}$$

$$P_l(\cos(\gamma)) = \frac{4\cdot\pi}{2\cdot\ell + 1}\cdot\sum_{j=-\ell}^{\ell}\left(Y(\ell, j, \Theta, \Phi)^*\cdot Y(\ell, j, \theta, \varphi)\right) \tag{25.19}$$

Angular moment theorem

A vector operator **J** is an angular momentum if its components are observables satisfying the following commutation relations:

$$\boxed{\mathbf{J} = \mathrm{J_x} \cdot \mathbf{i_x} + \mathbf{J_y} \cdot \mathbf{i_y} + \mathbf{J_z} \cdot \mathbf{i_z}} \tag{25.20}$$

$$[\ \mathbf{J_x}, \mathbf{J_y}\ ] = \mathrm{i} \cdot \hbar \cdot \mathbf{J_z} \tag{25.21}$$

$$[\ \mathbf{J_y}, \mathbf{J_z}\ ] = \mathrm{i} \cdot \hbar \cdot \mathbf{J_x} \tag{25.22}$$

$$[\ \mathbf{J_z}, \mathbf{J_x}\ ] = \mathrm{i} \cdot \hbar \cdot \mathbf{J_y} \tag{25.23}$$

If **a** and **b** are any two vectors (or any two vector operators that commute with each other and also with **J**) I get

$$[\ \mathbf{a} \cdot \mathbf{J}, \mathbf{b} \cdot \mathbf{J}\ ] = \mathrm{i} \cdot \hbar \cdot (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{J} \tag{25.24}$$

$$[\ \mathbf{J}, \mathbf{J}^2\ ] = 0 \tag{25.25}$$

$$[\ \mathrm{f}(\mathbf{J}_\alpha), \mathbf{J}^2\ ] = 0 \tag{25.26}$$

Hermitian conjugated operators: $\mathbf{J}_+ = \mathbf{J_x} + \mathrm{i} \cdot \mathbf{J_y}$ $\quad \mathbf{J}_- = \mathbf{J_x} - \mathrm{i} \cdot \mathbf{J_y}$

$$[\ \mathbf{J_z}, \mathbf{J}_+\ ] = \hbar \cdot \mathbf{J}_+ \tag{25.27}$$

$$[\ \mathbf{J_z}, \mathbf{J}_-\ ] = -\hbar \cdot \mathbf{J}_- \tag{25.28}$$

$$[\ \mathbf{J}_+, \mathbf{J}_-\ ] = 2 \cdot \hbar \cdot \mathbf{J_z} \tag{25.29}$$

Demonstration of (25.27), (25.28), (25.29)

$$[\ \mathbf{J}^2, \mathbf{J}_+\ ] = [\ \mathbf{J}^2, \mathbf{J}_-\ ] = [\ \mathbf{J}^2, \mathbf{J_z}\ ] = 0 \tag{25.30}$$

$$\mathbf{J}^2 = \frac{1}{2} \cdot (\mathbf{J}_+ \cdot \mathbf{J}_- + \mathbf{J}_- \cdot \mathbf{J}_+) + \mathbf{J_z}^2 \tag{25.31}$$

$$\mathbf{J}_- \cdot \mathbf{J}_+ = \mathbf{J}^2 - \mathbf{J_z} \cdot (\mathbf{J_z} + 1) \tag{25.32}$$

$$\mathbf{J}_+ \cdot \mathbf{J}_- = \mathbf{J}^2 - \mathbf{J_z} \cdot (\mathbf{J_z} - 1) \tag{25.33}$$

26 Charged Elemental Particle (Q) in an Electromagnetic Field

MKS-GAUSS

Electric field

The electric field is bounded to the vector potential by the relation:

$$\frac{\text{volt}}{\text{m}} \qquad \mathbf{E}(\mathbf{R},t) = -\nabla\,\varphi(\mathbf{R},t) - \frac{\partial}{\partial t}\mathbf{A}(\mathbf{R},t) \qquad \frac{\text{Wb}}{\text{m}\cdot\text{sec}} = 1\cdot\frac{\text{volt}}{\text{m}} \tag{26.1}$$

$$\frac{\partial}{\partial t}\mathbf{A}(\mathbf{R},t) = \nabla\,\mathbf{A}(\mathbf{R},t)\cdot\frac{\partial}{\partial t}\mathbf{R} = \mathbf{v}\cdot\nabla\,\mathbf{A}(\mathbf{R},t) \tag{26.2}$$

$$\frac{\text{volt}}{\text{m}} \qquad \mathbf{E}(\mathbf{R},t) = -\nabla\,\varphi(\mathbf{R},t) - \mathbf{v}\cdot\nabla\,\mathbf{A}(\mathbf{R},t) \qquad \frac{\text{Wb}}{\text{m}\cdot\text{sec}} = 1\cdot\frac{\text{volt}}{\text{m}} \tag{26.1'}$$

$$\mathbf{E}(\mathbf{R},t) = -\nabla\left(\varphi(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right)$$

verify

Consider the electric charge Q immersed in an electromagnetic field. It is subject to the Lorenz force:

$$\mathbf{F} = Q\cdot(\mathbf{E} + \mathbf{v}\times\mathbf{B}) \tag{26.3}$$

Substitute in it eq. 26.1) and the option 26.a1) (**Option 1)** . Results:

$$\mathbf{F} = m\cdot\mathbf{q''} = \mathbf{p'} = Q\cdot\left[-\nabla\,\varphi - \frac{\partial}{\partial t}\mathbf{A} + \mathbf{v}\times(\nabla\times\mathbf{A})\right] \tag{26.4}$$

$$\mathbf{v}\times(\nabla\times\mathbf{A}) = \nabla\,(\mathbf{v}\cdot\mathbf{A}) - \left[(\mathbf{v}\cdot\nabla)\cdot\mathbf{A} + (\mathbf{A}\cdot\nabla)\cdot\mathbf{v} + \mathbf{A}\times(\nabla\times\mathbf{v})\right] \tag{26.5}$$

$$\frac{\partial}{\partial t}\mathbf{A} = \mathbf{v}\cdot\nabla\,\mathbf{A} \tag{26.2}$$

$$\mathbf{F} = Q\cdot\left[-\nabla\,\varphi - \mathbf{v}\cdot\nabla\,\mathbf{A} + \nabla\,(\mathbf{v}\cdot\mathbf{A}) - \left[(\mathbf{v}\cdot\nabla)\cdot\mathbf{A} + (\mathbf{A}\cdot\nabla)\cdot\mathbf{v} + \mathbf{A}\times(\nabla\times\mathbf{v})\right]\right] \tag{26.6}$$

furthermore, collecting the gradient operators, I can write:

$$\mathbf{E}(\mathbf{R},t) = -\nabla\left(\varphi(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right) = -\nabla\left(\Phi_p\right) \tag{26.7}$$

so that I can define the scalar potential: $\boxed{\Phi_p(\mathbf{R},t) = V(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)}$ (26.8)

while the potential energy is $U(\mathbf{R},t) = Q\cdot\left(V(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right)$ $\qquad Q = \pm\, q_e$ (26.9)

which is useful to define the Lagrangian.

Lagrangian coordinates: $\mathbf{p} = m\cdot\mathbf{q'}$ $\qquad \mathbf{p'} = m\cdot\mathbf{q''}$ $\qquad \mathbf{q} = \mathbf{r}$ (26.10)

$$\mathbf{F} = m\cdot\mathbf{q''} = \mathbf{p'} \qquad \mathbf{q'} = \frac{\mathbf{p}}{m} \tag{26.11}$$

Cinematic moment (A is the potential vector)

$$T = \frac{\mathbf{p}^2}{2\cdot m} = \frac{\mathbf{p}\cdot m\cdot\mathbf{q'}}{2\cdot m} = \frac{\mathbf{p}\cdot\mathbf{q'}}{2} \tag{26.12}$$

$$U = Q\cdot\left(V(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right) + \Phi(\mathbf{r}) \tag{26.13}$$

Classical Lagrangian $\mathcal{L} = T - U = \dfrac{\mathbf{p}\cdot\mathbf{q'}}{2} - Q\cdot\left(V(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right) - \Phi(\mathbf{r}) \qquad U = T - \mathcal{L}$ (26.14)

$$\mathcal{L} = \frac{\mathbf{p}\cdot\mathbf{q'}}{2} - Q\cdot\left(V(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right) - \Phi(\mathbf{r}) = \frac{\mathbf{p}^2}{2\cdot m} - Q\cdot(V + \mathbf{v}\cdot\mathbf{A}) - \Phi(r) \tag{26.15}$$

Classical Hamiltonian in an electromagnetic field:

$$U = T - \mathcal{L} \qquad \mathcal{H} = T + U = 2\cdot T - \mathcal{L} = \mathbf{p}\cdot\mathbf{q'} - \frac{\mathbf{p}\cdot\mathbf{q'}}{2} + Q\cdot\left(V(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right) + \Phi(\mathbf{r}) \tag{26.16}$$

$$\mathcal{H} = \frac{\mathbf{p}\cdot\mathbf{q'}}{2} + Q\cdot\left(V(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right) + \Phi(\mathbf{r}) \tag{26.17}$$

Classical Lagrangian for one electron (**Φ**=0, Q=-q_e) in an electromagnetic field:

$$\mathcal{L} = \frac{\mathbf{p}\cdot\mathbf{q'}}{2} + q_e\cdot\left(V(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right) \tag{26.18}$$

Classical Hamiltonian for one electron (**Φ**=0, Q=-q_e) in an electromagnetic field:

$$\mathcal{H} = \frac{\mathbf{p}\cdot\mathbf{q'}}{2} - q_e\cdot\left(V(\mathbf{R},t) + \mathbf{v}\cdot\mathbf{A}(\mathbf{R},t)\right) + \Phi(\mathbf{r}) \tag{26.19}$$

Scalar potential due to electrostatic field $V(\mathbf{r}) = -\int \mathbf{E}(\mathbf{r})\, d\mathbf{r}$, or $\mathbf{E}(r) = -\nabla V(r)$ (26.20)

The Potential due to non electromagnetic forces is indicated with $\Phi(\mathbf{r})$

Electromagnetic vector potential $\mathbf{A}$, magnetic induction $\mathbf{B} = \nabla \times \mathbf{A}$ (T) . In a system of currents, A is the solution of t Helmholtz equation

$$\nabla^2 \mathbf{A}(x,y,z) + k^2\cdot\mathbf{A}(x,y,z) = -\mathbf{J}_{\boldsymbol{\sigma}}(x,y,z), \qquad k^2 = \omega^2\cdot\mu\cdot\varepsilon \tag{26.21}$$

$$\mathbf{A}(x,y,z) = \frac{1}{4\cdot\pi}\int\int\int \mathbf{J}(p_1)\cdot\frac{e^{-i\cdot(|p-p_1|)}}{|p-p_1|}\, dx\, dy\, dz \tag{26.22}$$

Apply the quantization rules to the classical Hamiltonian of one electron (**Φ**=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
$\mathbf{p}$	$\leftrightarrow -i\cdot\hbar\cdot\nabla$,
$\mathbf{q'}$	$\leftrightarrow -i\cdot\dfrac{\hbar}{m}\cdot\nabla$
$\mathbf{L} = \mathbf{r}\times\mathbf{p}$	$\leftrightarrow -i\cdot\hbar\cdot\mathbf{r}\times\nabla$,
$\mathbf{l_x}$	$\leftrightarrow -i\cdot\hbar\cdot\left(y\cdot\dfrac{\partial}{\partial z} - z\cdot\dfrac{\partial}{\partial y}\right)$,
$\mathbf{l_y}$	$\leftrightarrow -i\cdot\hbar\cdot\left(z\cdot\dfrac{\partial}{\partial x} - x\cdot\dfrac{\partial}{\partial z}\right)$,
$\mathbf{l_z}$	$\leftrightarrow -i\cdot\hbar\cdot\left(x\cdot\dfrac{\partial}{\partial y} - y\cdot\dfrac{\partial}{\partial x}\right)$,

$$\mathbf{p}^2 \leftrightarrow -\hbar^2 \cdot \Delta,$$

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

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

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

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

$$\mathbf{s}\cdot\mathbf{p} \leftrightarrow \nabla\times \qquad \text{A. M. 551}$$

***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 $E = T + U = \mathcal{H}$. In QM, to E and $\mathcal{H}$ correspond to each an operators acting on a ket:

$$\mathbf{E} \,|\, \Psi > = \mathbf{H} \,|\, \Psi >. \qquad (26.24\,)$$

Namely, applying the previous substitutions rules, I get (vector operators are written with **bold** fonts):

$$\mathcal{H} = \frac{\mathbf{p}^2}{2\cdot m} - q_e\cdot\left(V + \frac{m\cdot\mathbf{v}\cdot\mathbf{A}(\mathbf{q},t)}{m}\right) + \Phi(\mathbf{r}) = \frac{\mathbf{p}^2}{2\cdot m} - q_e\cdot V - \frac{q_e\cdot\mathbf{p}\cdot\mathbf{A}(\mathbf{q},t)}{m} + \Phi(\mathbf{r}) \qquad (26.23)$$

Classical Hamiltonian $\leftrightarrow$ QM Hamiltonian (26.25)

$\downarrow$ $\downarrow$

$$\mathcal{H} = \frac{\mathbf{p}^2}{2\cdot m} - q_e\cdot V - \frac{q_e\cdot\mathbf{p}\cdot\mathbf{A}(\mathbf{q},t)}{m} + \Phi(\mathbf{r}) \quad \leftrightarrow \quad \mathbf{H} = -\frac{\hbar^2}{2\cdot m}\cdot\nabla^2 + \frac{i\cdot q_e\cdot\hbar}{m}\cdot\mathbf{A}\cdot\nabla - q_e\cdot V + \Phi(\mathbf{r}) \qquad (26.26)$$

in fact for the scalar product between $\mathbf{p}$ and $\mathbf{A}$, I can write $\mathbf{p}\cdot\mathbf{A} = \mathbf{A}\cdot\mathbf{p} \leftrightarrow -i\cdot\hbar\cdot\mathbf{A}\cdot\nabla$ (26.27)

classical Hamiltonian of the electron: $\mathcal{H} = \frac{\mathbf{p}^2}{2\cdot m} + \frac{\mathbf{A}^2\cdot q_e^{\,2}}{2\cdot c^2\cdot m} + \frac{\mathbf{A}\cdot\mathbf{p}\cdot q_e}{c\cdot m} - q_e\cdot V(\mathbf{r}) + \Phi(\mathbf{r})$ (26.28)

QM Hamiltonian operator $\mathbf{H} = -\frac{\hbar^2}{2\cdot m}\cdot\nabla^2 + \frac{i\cdot q_e\cdot\hbar}{2\cdot m\cdot c}\cdot(\nabla\bullet\mathbf{A} + \mathbf{A}\cdot\nabla) + \frac{q_e^{\,2}}{2\cdot m\cdot c^2}\cdot\mathbf{A}^2 - q_e\cdot V + \Phi$ (26.29)

H+H^†

Probability current density $\mathbf{J} = \frac{\hbar}{2\cdot m\cdot i}\cdot\left(\overline{\Psi}\cdot\nabla\,\Psi - \Psi\cdot\nabla\,\overline{\Psi} - 2i\cdot\frac{q_e}{\hbar\cdot c}\cdot\mathbf{A}\cdot\overline{\Psi}\cdot\Psi\right)$ (26.30)

or $\mathbf{J} = \frac{\hbar}{2\cdot m\cdot i}\cdot\left[\left(\overline{\Psi}\cdot\nabla\,\Psi - \Psi\cdot\nabla\,\overline{\Psi}\right) - \frac{q_e}{m\cdot c}\cdot\overline{\Psi}\cdot\Psi\cdot\mathbf{A}\right]$ (26.31)

varie

Remark on parity

Remark on parity [4]

$$\left(\frac{-\hbar^2}{2\cdot m}\cdot\Delta + V(x)\right) | \psi > = E | \psi >$$

$$V(x) = \frac{\hbar^2}{2\cdot m}\cdot U(x) \qquad E = \frac{\hbar^2}{2\cdot m}\cdot\varepsilon$$

$$\left(\frac{-\hbar^2}{2\cdot m}\cdot\Delta + \frac{\hbar^2}{2\cdot m}\cdot U(x)\right) | \psi > = \frac{\hbar^2}{2\cdot m}\cdot\varepsilon | \psi >$$

$$(-\Delta + U(x)) | \psi > = \varepsilon | \psi >$$

$$\Delta | \psi > = (U - \varepsilon) | \psi >$$

$$\frac{\partial^2}{\partial x^2}\psi(x) - (U - \varepsilon)\cdot\psi(x) = 0$$

If the potential U is even, that is to say if $U(x) = U(-x)$, the Schrödinger Hamiltonian doesn't change when I replace 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:

$$\mathbf{H} | \psi(x) > = E | \psi(x) > \quad \rightarrow \quad \mathbf{H} | \psi(-x) > = E | \psi(-x) >$$

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 always even. Increasing the eigenvalues of the energy, alternately the eigenfunctions are even and odd.
2) **E is degenerate**, then each eigenfunction ψ 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 degener 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 symmet properties. Parity is an example of this.
Consider the observable parity indicated with **P**:

$$\mathbf{P} | \psi(x) > = | \psi(-x) >,$$

P is Hermitian

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

$$\mathbf{P}^2 = 1.$$

The eigenvalues λ of $\mathbf{P} | \psi(q) > = \lambda | \psi(-q) >$ 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:

$$[\mathbf{P}, \mathbf{H}] = 0.$$

If $\mathbf{H}\left(\frac{\hbar}{i}\cdot\frac{d}{dq}, q\right) = \mathbf{H}\left(-\frac{\hbar}{i}\cdot\frac{d}{dq}, -q\right) \Rightarrow \forall | \psi(q) >,$

$$\mathbf{PH} | \psi(q) > = \mathbf{H}\left(-\frac{\hbar}{i}\cdot\frac{d}{dq}, -q\right) | \psi(-q) > = \mathbf{H}\left(\frac{\hbar}{i}\cdot\frac{d}{dq}, q\right) | \psi(q) > = \mathbf{HP} | \psi(q) >.$$

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.

Remark on parity

27 Pauli Matrices [4]

Hermitian $\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ (27.1)

Anti Hermitian $i \cdot \sigma_1 = \begin{pmatrix} 0 & j \\ j & 0 \end{pmatrix}$ $i \cdot \sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ $i \cdot \sigma_3 = \begin{pmatrix} j & 0 \\ 0 & -j \end{pmatrix}$ (27.2)

Calculations

28 Statistical Mixtures [4]

Statistical mixture of states: the dynamical state of the system ***is incompletely known***. One assign 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 $p_1, p_2, \ldots, p_n$ to find itself in the dynamical states represented by the ket vectors $|1\rangle, |2\rangle, \ldots, |n\rangle$. In other words the dynamic 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 **A**. *After n measurement* I have the average value of the n results indicated with $\langle \mathbf{A} \rangle_n$.

$$\langle \mathbf{A} \rangle_n = \frac{\left(\langle n | A | n \rangle\right)}{\langle n | n \rangle} \tag{28.1}$$

For normalized eigenvectors I have $\langle n | n \rangle = 1$, so that: $\langle \mathbf{A} \rangle_n = \langle n | A | n \rangle$, while

$$\langle \mathbf{A} \rangle = \sum_n \left[p_n \cdot \left(\langle \mathbf{A} \rangle_n\right)\right] = \sum_n \left(p_n \cdot \langle n | A | n \rangle\right) \tag{28.2}$$

in fact if I indicate with a_{ij} the result of each measurement, I have: $\langle \mathbf{A} \rangle_i = \dfrac{\sum_j a_{ij}}{n_i} = \langle i | \mathbf{A} | i \rangle \quad \left| \, | i \rangle \right| = 1$

$$\langle \mathbf{A} \rangle = \frac{\sum_i \sum_j a_{ij}}{\sum_k n_k} = \frac{\sum_i \left[n_i \cdot \left(\langle \mathbf{A} \rangle_i\right)\right]}{\sum_k n_k} = \sum_i \left[\frac{n_i}{\sum_k n_k} \cdot \left(\langle \mathbf{A} \rangle_i\right)\right] \tag{28.3}$$

define the statistical weight as: $$\frac{n_i}{\sum_k n_k} = p_i \tag{28.4}$$

so that $$\langle \mathbf{A} \rangle = \sum_n \left[p_n \cdot \left(\langle \mathbf{A} \rangle_n\right)\right] = \sum_n \left(p_n \cdot \langle n | \mathbf{A} | n \rangle\right) \tag{28.5}$$

the statistical weigh is given by the projector: $$\mathbf{p_n} = | n \rangle \langle n | \qquad p_n \geq 0 \qquad \sum_n p_n = 1 \tag{28.6}$$

$$\mathbf{P} = \sum_n \mathbf{p_n} = \sum_n | n \rangle \langle n | \tag{28.7}$$

Consider the projector $\mathbf{P_n} = | n \rangle \langle n |$

$$\mathrm{Tr}\left(\mathbf{P_n}\right) = 1$$

$$\mathrm{Tr}\left(\mathbf{P_n} \cdot \mathbf{A}\right) = \mathrm{Tr}\left(\mathbf{P_n}^2 \cdot \mathbf{A}\right) = \mathrm{Tr}\left(\mathbf{P_n} \cdot \mathbf{A} \cdot \mathbf{P_n}\right)$$

$$\mathrm{Tr}(\mathbf{P_n}\cdot\mathbf{A}\cdot\mathbf{P_n}) = \mathrm{Tr}(|\,n><n\,|\cdot\mathbf{A}\cdot|\,n><n\,|) = <n\,|\,\mathbf{A}\,|\,n>\cdot\mathrm{Tr}(|\,n><n\,|) = <n\,|\,\mathbf{A}\,|\,n>$$

If **A**=1 $\quad \mathrm{Tr}(\mathbf{P_n}) = <n\,|\,n> = 1$

$$<\mathbf{A}> = \sum_n \left[p_n\cdot(<\mathbf{A}>_n)\right] = \sum_n (p_n\cdot <n\,|\,\mathbf{A}\,|\,n>) = \sum_n (p_n\cdot\mathrm{Tr}(P_n\cdot\mathbf{A})) = \sum_n (p_n\cdot\mathrm{Tr}(|\,n><n\,|\cdot\mathbf{A}))$$

Statistic Operator or Density Operator: $\rho = \sum_n |\,n>p_n<n\,| \qquad <n\,|\,n> = 1$ (28.8)

Knowing ρ, I can find the statistical distribution of the results of measurement of **A**

The dynamical state of the system is represented usefully by the statistical mixture of ket vectors.

p_n is a statistical weight $\sum_n p_n = 1$ (28.9)

$$\rho > 0 \tag{28.10}$$

$$\rho = \rho^{\dagger} \tag{28.11}$$

$$\mathrm{Tr}(\rho\cdot\mathbf{A}) = <\mathbf{A}> \qquad A = 1 \qquad \mathrm{Tr}(\rho) = 1$$

Operator trace $\mathrm{Tr}(\rho) = 1$ (28.12)

$$\mathrm{Tr}(\rho^2) \le 1 \tag{28.13}$$

Average value of the observable **A**: $<\mathbf{A}> = \mathrm{Tr}(\rho\cdot\mathbf{A}) = <n\,|\,\mathbf{A}\,|\,n>$ (28.14)

Average value of the function of the observable F(**A**): $<F(\mathbf{A})> = \mathrm{Tr}(\rho\cdot F(\mathbf{A}))$ (28.15)

The probability that the result of measurement belong to domain D of the spectrum of **A** is

$$w_D = <\mathbf{P_D}> = \mathrm{Tr}(\rho\cdot\mathbf{P_D}), \tag{28.16}$$

where $\mathbf{P_D}$ is the projector upon the subspace spanned by the eigenvectors of **A**.

The probability of finding the system in the quantum state represented by the normalize ket $|\,x>$, is:

$$w_x = \mathrm{Tr}(\rho\cdot|\,x><x\,|) \tag{28.17}$$

Two statistical mixtures possessing the same density operator, are identical.

The Schrödinger equation of the Density Operator: $\boxed{i\cdot\hbar\cdot\frac{\partial}{\partial t}\rho = [\,\mathbf{H},\rho\,]}$ (28.18)

$$i\cdot\hbar\cdot\frac{\partial}{\partial t}\rho_{k,\ell} = <k\,|\,[\,\mathbf{H},\rho\,]\,|\,\ell> \tag{28.19}$$

$$\mathbf{H} = \mathbf{H}^{\dagger} \;\Rightarrow\; \frac{\partial}{\partial t}\rho_{k,\ell} = -i\cdot\omega_{k,\ell}\cdot\rho_{k,\ell} \tag{28.20}$$

$$\omega_{k,\ell} = \frac{E_k - E_\ell}{\hbar} \tag{28.21}$$

$$\rho(t)_{k,\ell} = \rho(0)_{k,\ell}\cdot e^{-i\cdot\omega_{k,\ell}\cdot(t-t_0)} \qquad (28.22)$$

for k=ℓ $\quad \omega_{k,k} = \dfrac{E_k - E_k}{\hbar} = 0 \qquad \rho_{k,k} = \rho_{k,k}(0)$ 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 $|\chi>$ can be represented as the only state of a statistical mixture; so that its density operator is

$$\rho_\chi = |\chi><\chi|$$

$$\rho_\chi^{\ 2} = \rho_\chi .$$

If a density operator is a projector, than it represents a pure state.
Since a density operator can be represented by the superposition

$$\rho = \sum_n |n> p_n < n| ,$$

in order that it represents a pure state it is necessary and sufficient that each $|n>$ be equal to each other to within a phase.
Furthermore if $\mathrm{Tr}(\rho^2) = 1$, than the density operator represents a pure state.

The state of a quantum system whose Hamiltonian is **H,** in thermodynamic equilibrium at temperature T is representec the operator

$$\rho = N\cdot e^{-\frac{\mathbf{H}}{k_B\cdot T}} ,$$

where N is a normalization constant such that Tr($\boldsymbol{\rho}$)=1.
System entropy

$$S = -k\cdot\mathrm{Tr}(\rho\cdot\ln(\rho))$$

29 Hamiltonian for macroscopic systems and small interactions close to equilibrium

$$\mathbf{H} = \mathbf{H_0} + \mathbf{H_{int}} + \mathbf{H_r} \tag{29.1}$$

Unperturbed Hamiltonian $\mathbf{H_0}$

Interaction Hamiltonian $\mathbf{H_{int}}$

Relaxation Hamiltonian $\mathbf{H_r}$

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} \rho_{k,\ell} = \left([\, \mathbf{H_0}, \rho \,] \right)_{k,\ell} + \left([\, \mathbf{H_{int}}, \rho \,] \right)_{k,\ell} + \left([\, \mathbf{H_r}, \rho \,] \right)_{k,\ell}$$

$$\mathbf{H_0} > \mathbf{H_{int}} \wedge \mathbf{H_0} > \mathbf{H_r} \;\Rightarrow\; -i \cdot \hbar \cdot \frac{\partial}{\partial t} \rho_{k,\ell} = \left([\, \mathbf{H_r}, \rho \,] \right)_{k,\ell} \quad k \neq \ell$$

$$\mathbf{H_1} = \mathbf{H_0} + \mathbf{H_{int}}$$

$$\begin{pmatrix} i \cdot \hbar \cdot \frac{\partial}{\partial t} \rho_{k,\ell} \\ i \cdot \hbar \cdot \frac{\partial}{\partial t} \rho_{k,\ell} \end{pmatrix} = \begin{bmatrix} i \cdot \hbar \cdot \frac{\rho_{k,\ell}}{\tau_{k,\ell}} \\ \left([\, \mathbf{H_1}, \rho \,] \right)_{k,\ell} + i \cdot \frac{\hbar}{T_1} \cdot \left(\rho_{\mathbf{e}_{k,k}} - \rho_{k,k} \right) \end{bmatrix}$$

If $\mathbf{H_{int}} = 0 \Rightarrow \left([\, \mathbf{H_0}, \rho \,] \right)_{k,k} = C_0 \Rightarrow W_{n,k} \cdot \rho_{\mathbf{e}_{n,n}} = W_{k,n} \cdot \rho_{\mathbf{e}_{k,k}}$ ***this is the "detailed balance principle"***

30 Algebra of the one-dimensional harmonic oscillator [6]

The classical Hamiltonian of a simple (without damping) mechanical oscillator (composed by a mass m) is:

$$\mathcal{H} = \frac{1}{2}\cdot m\cdot x'^2 + \frac{m\cdot\omega^2}{2}\cdot x^2 \qquad (30.1)$$

considering the Lagrangian conjugated momenta, I can write $\mathcal{H} = \frac{1}{2}\cdot m\cdot q'^2 + \frac{1}{2}\cdot m\cdot\omega^2\cdot q^2$ (30.1)

$$\text{where: } x' = q' \qquad p = m\cdot q' \qquad q'^2 = \left(\frac{p}{m}\right)^2 = \frac{p^2}{m^2} \qquad (30.2)$$

so that the Hamiltonian takes the form: $\mathcal{H} = \frac{1}{2\cdot m}\cdot\left(p^2 + m^2\cdot\omega^2\cdot q^2\right)$ (30.3)

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: $\mathcal{H} = \frac{1}{2\cdot m}\cdot\left(p^2 + m^2\cdot\omega^2\cdot q^2\right) \quad\leftrightarrow\quad \mathbf{H} = \frac{-\hbar^2}{2\cdot m}\cdot\Delta + \frac{m\cdot\omega^2}{2}\cdot q^2$ (30.4)

The Schrödinger equation of motion is:

$$i\cdot\hbar\cdot\frac{\partial}{\partial t}\left|\,\Psi\right\rangle = \mathbf{H}\left|\,\Psi\right\rangle \qquad (30.5)$$

that is: $i\cdot\hbar\cdot\frac{\partial}{\partial t}\left|\,\Psi\right\rangle = \left(\frac{-\hbar^2}{2\cdot m}\cdot\Delta + \frac{m\cdot\omega_0^{\,2}}{2}\cdot q^2\right)\left|\,\Psi\right\rangle$ (30.6)

When the system is in a stationary state of energy E, I get $\left|\,\Psi\right\rangle = e^{-i\cdot\frac{E\cdot t}{\hbar}}\left|\,\psi\right\rangle$

$$E\left|\,\psi\right\rangle = \mathbf{H}\left|\,\psi\right\rangle$$

Commutator [q,p] calculations

with the previous assumption I want see how the Hamiltonia **H** is related to the Lagrangian variables position **q** and conjugated momentum **p**. I found that:

$$[\,\mathbf{q},\mathbf{p}\,] = i\cdot\hbar \qquad (30.7)$$

Define the new operators: $\mathbf{q} = \sqrt{\frac{\hbar}{m\cdot\omega}}\cdot\mathbf{Q}$ and $\mathbf{p} = \sqrt{\hbar\cdot m\cdot\omega}\cdot\mathbf{P}$ [6] (30.8) substituting in (30.7) 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 $\boxed{[\,\mathbf{Q},\mathbf{P}\,] = i\cdot\mathbf{I}}$ (30.9)

Furthermore substituting (30.8) into the Hamiltonian (30.4), results:

$$\mathbf{H} = \frac{1}{2\cdot m}\cdot\left(\mathbf{p}^2 + m^2\cdot\omega^2\cdot\mathbf{q}^2\right) = \frac{1}{2\cdot m}\cdot\left(\hbar\cdot m\cdot\omega\cdot\mathbf{P}^2 + m^2\cdot\omega^2\cdot\frac{\hbar}{m\cdot\omega}\cdot\mathbf{Q}^2\right)$$

$$\mathbf{H} = \frac{1}{2\cdot m}\cdot\left(\hbar\cdot m\cdot\omega\cdot\mathbf{P}^2 + \hbar\cdot m\cdot\omega\cdot\mathbf{Q}^2\right) = \frac{\hbar\cdot\omega}{2}\cdot\left(\mathbf{P}^2 + \mathbf{Q}^2\right) \quad (30.10)$$

namely: $\boxed{\mathbf{H} = \frac{\hbar\cdot\omega}{2}\cdot\left(\mathbf{P}^2 + \mathbf{Q}^2\right)}$ (30.11)

I place: $\mathbf{H} = \hbar\cdot\omega\cdot\mathbf{H_0}$

so that, thanks to (30.11), I get: $\mathbf{H_0} = \frac{1}{2}\cdot\left(\mathbf{P}^2 + \mathbf{Q}^2\right)$ (30.12)

(Q+iP)(Q-iP)

(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 (30.12) can be rewritten as: $\mathbf{H_0} = \frac{1}{2}\cdot\left[(\mathbf{Q} + i\cdot\mathbf{P})\cdot(\mathbf{Q} - i\cdot\mathbf{P}) - \mathbf{I}\right]$

A further simplification is reached with defining the three new following QM operators:

(Ladder) operator: $\mathbf{a} = \frac{1}{\sqrt{2}}\cdot(\mathbf{Q} + i\cdot\mathbf{P})$ (30.13)

(Ladder) operator: $\mathbf{a}^\dagger = \frac{1}{\sqrt{2}}\cdot(\mathbf{Q} - i\cdot\mathbf{P})$ (30.14)

Since $\mathbf{a} \neq \mathbf{a}^\dagger$ they aren't Hermitian.

Number operator: $\mathbf{N} = \mathbf{a}^\dagger\cdot\mathbf{a} \qquad \mathbf{N}^\dagger = \mathbf{a}\cdot\mathbf{a}^\dagger$ (30.15)

Complex conjugated of **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 **a** and $\mathbf{a}^\dagger$ are:

the sum: $\mathbf{a}^\dagger + \mathbf{a} = \frac{1}{\sqrt{2}}\cdot(\mathbf{Q} - i\cdot\mathbf{P} + \mathbf{Q} + i\cdot\mathbf{P}) = \sqrt{2}\cdot\mathbf{Q}$ (30.16)

$\boxed{\mathbf{Q} = \frac{1}{\sqrt{2}}\cdot\left(\mathbf{a}^\dagger + \mathbf{a}\right)}$ (30.17)

the difference: $\mathbf{a}^\dagger - \mathbf{a} = \frac{1}{\sqrt{2}}\cdot\left[\mathbf{Q} - i\cdot\mathbf{P} - (\mathbf{Q} + i\cdot\mathbf{P})\right] = \sqrt{2}\cdot i\cdot\mathbf{P}$ (30.18)

$$\boxed{\mathbf{P} = \frac{1}{\sqrt{2}}\cdot\left(\mathbf{a}^{\dagger} - \mathbf{a}\right)} \qquad (30.19)$$

Product: $$\mathbf{a}\cdot\mathbf{a}^{\dagger} = \frac{1}{2}\cdot(\mathbf{Q} + i\cdot\mathbf{P})\cdot(\mathbf{Q} - i\cdot\mathbf{P}) = \frac{1}{2}\cdot\left(\mathbf{P}^2 + \mathbf{Q}^2 + \mathbf{I}\right) = \mathbf{H_0} + \frac{1}{2}\cdot\mathbf{I} \qquad (30.20)$$

$$\mathbf{a}^{\dagger}\cdot\mathbf{a} = \frac{1}{2}\cdot(\mathbf{Q} - i\cdot\mathbf{P})\cdot(\mathbf{Q} + i\cdot\mathbf{P}) = \frac{1}{2}\cdot\left(\mathbf{Q}^2 + \mathbf{P}^2 - \mathbf{I}\right) = \mathbf{H_0} - \frac{1}{2}\cdot\mathbf{I} \qquad (30.21)$$

The commutator between $\mathbf{a}$ and $\mathbf{a}^{\dagger}$ can be found using (30.20) and (30.21):

$$[\,\mathbf{a}, \mathbf{a}^{\dagger}\,] = \mathbf{a}\cdot\mathbf{a}^{\dagger} - \mathbf{a}^{\dagger}\cdot\mathbf{a} = \mathbf{H_0} + \frac{1}{2}\cdot\mathbf{I} - \left(\mathbf{H_0} - \frac{1}{2}\cdot\mathbf{I}\right) = \mathbf{I}$$

$$[\,\mathbf{a}, \mathbf{a}^{\dagger}\,] = \mathbf{I} \qquad [\,\mathbf{a}^{\dagger}, \mathbf{a}\,] = -\mathbf{I} \qquad (30.22)$$

From (30.21) I get the operator number as a function of the Hamiltonian $\mathbf{H}$:

$$\mathbf{N} = \mathbf{a}^{\dagger}\cdot\mathbf{a} = \mathbf{H_0} - \frac{1}{2}\cdot\mathbf{I} \qquad (30.23)$$

that is the Hamiltonian takes the form $\boxed{\mathbf{H_0} = \mathbf{N} + \frac{1}{2}\cdot\mathbf{I}}$ $\qquad \mathbf{H} = \hbar\cdot\omega\cdot\mathbf{H_0} \qquad (30.24)$

The Hamiltonian can also take other forms, in fact consider the commutator:

$$[\,\mathbf{a}, \mathbf{a}^{\dagger}\,] = \mathbf{a}\cdot\mathbf{a}^{\dagger} - \mathbf{a}^{\dagger}\cdot\mathbf{a} = \mathbf{N}^{\dagger} - \mathbf{N} \qquad (30.25)$$

From (30.20) , I have: $$\mathbf{N}^{\dagger} = \mathbf{a}\cdot\mathbf{a}^{\dagger} = \mathbf{H_0} + \frac{1}{2}\cdot\mathbf{I} \qquad (30.26)$$

namely: $$\boxed{\mathbf{N}^{\dagger} = \mathbf{H_0} + \frac{1}{2}\cdot\mathbf{I}} \qquad (30.27)$$

Calculation of the commutator $[\,\mathbf{N}, \mathbf{a}\,] = [\,\mathbf{a}^{\dagger}\cdot\mathbf{a}, \mathbf{a}\,] = \mathbf{a}^{\dagger}\cdot\mathbf{a}\cdot\mathbf{a} - \mathbf{a}\cdot\mathbf{a}^{\dagger}\cdot\mathbf{a}$ $\qquad \mathbf{a}^{\dagger}\cdot\mathbf{a} = \mathbf{a}\cdot\mathbf{a}^{\dagger} - \mathbf{I}$

[N,a]

the result is: $$\boxed{[\,\mathbf{N}, \mathbf{a}\,] = -\mathbf{a}} \qquad (30.28)$$

I adopt the same procedure to calculate the commutator $[\,\mathbf{N}, \mathbf{a}^{\dagger}\,]$, namely: $\mathbf{a}\cdot\mathbf{a}^{\dagger} = \mathbf{a}^{\dagger}\cdot\mathbf{a} + \mathbf{I}$

[N,a†]

the result is: $$\boxed{[\,\mathbf{N}, \mathbf{a}^{\dagger}\,] = \mathbf{a}^{\dagger}} \qquad (30.29)$$

Can be useful to calculate the following difference using (30.27) and (30.24):

$$\mathbf{N}^{\dagger} - \mathbf{N} = \mathbf{a}\cdot\mathbf{a}^{\dagger} - \mathbf{a}^{\dagger}\cdot\mathbf{a} = \mathbf{H_0} + \frac{1}{2}\cdot\mathbf{I} - \mathbf{H_0} + \frac{1}{2}\cdot\mathbf{I} = \mathbf{I}$$

$$\mathbf{N} = \mathbf{N}^{\dagger} - \mathbf{I}$$

$$\mathbf{N}^{\dagger} = \mathbf{N} + \mathbf{I}$$

$$\mathbf{N}^{\dagger} - \mathbf{N} = \mathbf{I}$$

The sum: $\mathbf{N}^{\dagger} + \mathbf{N} = \mathbf{H_0} + \frac{1}{2}\cdot\mathbf{I} + \mathbf{H_0} - \frac{1}{2}\cdot\mathbf{I} = 2\cdot\mathbf{H_0}$

$$\mathbf{H_0} = \frac{1}{2}\cdot\left(\mathbf{N}^{\dagger} + \mathbf{N}\right) \qquad (30.30)$$

The Hamiltonian as a function of $\mathbf{a}$ and $\mathbf{a}^{\dagger}$:

from (30.28): $\boxed{\mathbf{H_0} = \frac{1}{2}\cdot\left(\mathbf{N}^{\dagger} + \mathbf{N}\right) = \frac{1}{2}\cdot\left(\mathbf{a}^{\dagger}\cdot\mathbf{a} + \mathbf{a}\cdot\mathbf{a}^{\dagger}\right)}$ (30.31)

from (30.27) I get: $\boxed{\mathbf{H_0} = \mathbf{N}^{\dagger} - \frac{1}{2}\cdot\mathbf{I}}$ $\quad \mathbf{H} = \hbar\cdot\omega\cdot\mathbf{H_0}$ (30.32)

$$i\cdot\hbar\cdot\frac{\partial}{\partial t}\,|\,\psi> = \mathbf{H_0}\,|\,\psi> = \left(\mathbf{N}^{\dagger} - \frac{1}{2}\cdot\mathbf{I}\right)|\,\psi>$$

The ***Schrödinger equation*** of motion is: $\boxed{\frac{\partial}{\partial t}\,|\,\psi> = \frac{-i}{\hbar}\cdot\left(\mathbf{N}^{\dagger} - \frac{1}{2}\cdot\mathbf{I}\right)|\,\psi>}$ (30.33)

$$i\cdot\hbar\cdot\frac{\partial}{\partial t}\,|\,\psi> = \mathbf{H_0}\,|\,\psi> = \left(\mathbf{N} + \frac{1}{2}\cdot\mathbf{I}\right)|\,\psi>$$

$$i\cdot\hbar\cdot\frac{\partial}{\partial t}\,|\,\psi> = \left(\mathbf{N} + \frac{1}{2}\cdot\mathbf{I}\right)|\,\psi>$$

The ***Schrödinger equation*** of motion is: $\boxed{\frac{\partial}{\partial t}\,|\,\psi> = \frac{-i}{\hbar}\cdot\left(\mathbf{N} + \frac{1}{2}\cdot\mathbf{I}\right)|\,\psi>}$ (30.34)

$$i\cdot\hbar\cdot\frac{\partial}{\partial t}\,|\,\psi> = \mathbf{H_0}\,|\,\psi> = \frac{1}{2}\cdot\left(\mathbf{a}\cdot\mathbf{a}^{\dagger} + \mathbf{a}^{\dagger}\cdot\mathbf{a}\right)|\,\psi>$$

The ***Schrödinger equation*** of motion is: $\boxed{\frac{\partial}{\partial t}\,|\,\psi> = \frac{-i}{2\cdot\hbar}\cdot\left(\mathbf{a}^{\dagger}\cdot\mathbf{a} + \mathbf{a}\cdot\mathbf{a}^{\dagger}\right)|\,\psi>}$ (30.35)

31 Eigenvalues and eigenvectors of the energy associated with H and N [6]

Assuming that there exists at least one eigenket of **N** in Hilbert space $\mathbb{H}$, I can write:

$$\mathbf{N}\,|\,\varphi_{\nu}> = \nu\,|\,\varphi_{\nu}>, \qquad (31.1)$$

where $\mathbf{N} = \mathbf{a}^{\dagger}\cdot\mathbf{a}$ and $<\varphi_{\nu}\,|\,\varphi_{\nu}> = \lambda_{\nu}$, that is the ket $|\,\varphi_{\nu}>$ isn't normalized.

Now write the eigenvalue equation for the ket: $\mathbf{a}\,|\,\varphi_{\nu}>$ keeping in mind (30.28) $\boxed{[\,\mathbf{N},\mathbf{a}\,] = -\mathbf{a}}$: (31.2)

$$[\,\mathbf{N},\mathbf{a}\,] = \mathbf{N}\cdot\mathbf{a} - \mathbf{a}\cdot\mathbf{N} \qquad \mathbf{N}\cdot\mathbf{a} = [\,\mathbf{N},\mathbf{a}\,] + \mathbf{a}\cdot\mathbf{N} = -\mathbf{a} + \mathbf{a}\cdot\mathbf{N} = \mathbf{a}\cdot(\mathbf{N} - \mathbf{I})$$

$$\mathbf{N}\cdot\mathbf{a}\,|\,\varphi_{\nu}> = \mathbf{a}\cdot(\mathbf{N} - \mathbf{I})\,|\,\varphi_{\nu}> = (\nu - 1)\cdot\mathbf{a}\,|\,\varphi_{\nu}>, \qquad (31.3)$$

Knowing that [eq. (30.22)]: $[\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{a}\cdot\mathbf{a}^\dagger - \mathbf{a}^\dagger\cdot\mathbf{a} = \mathbf{I}$

it follows that: $\mathbf{a}^\dagger\cdot\mathbf{a} = \mathbf{a}\cdot\mathbf{a}^\dagger - \mathbf{I}$ (31.4)

apply **a** on the right of (31.4) : $\mathbf{a}^\dagger\cdot\mathbf{a}\cdot\mathbf{a} = \left(\mathbf{a}\cdot\mathbf{a}^\dagger - \mathbf{I}\right)\cdot\mathbf{a} = \mathbf{a}\cdot\mathbf{a}^\dagger\cdot\mathbf{a} - \mathbf{a} = \mathbf{a}\cdot\left(\mathbf{a}^\dagger\cdot\mathbf{a} - \mathbf{I}\right)$ (31.5)

so that eq. (31.3) can be rewritten as: $\mathbf{N}\cdot\mathbf{a} \mid \varphi_\nu > = \mathbf{a}^\dagger\cdot\mathbf{a}\cdot\mathbf{a} \mid \varphi_\nu > = \left(\mathbf{a}\cdot\mathbf{a}^\dagger - \mathbf{I}\right)\cdot\mathbf{a} \mid \varphi_\nu >$

therefore: $\mathbf{N}\cdot\mathbf{a} \mid \varphi_\nu > = \mathbf{a}\cdot\left(\mathbf{a}^\dagger\cdot\mathbf{a} - \mathbf{I}\right) \mid \varphi_\nu > = \mathbf{a}\cdot(\mathbf{N} - \mathbf{I}) \mid \varphi_\nu >$

resulting: $\boxed{\mathbf{N}\cdot\mathbf{a} = \mathbf{a}\cdot(\mathbf{N} - \mathbf{I})}$ (31.6)

the eigenvalues equation is: $\mathbf{a}\cdot(\mathbf{N} - \mathbf{I}) \mid \varphi_\nu > = \mathbf{a}\cdot(\nu - 1) \mid \varphi_\nu > = (\nu - 1)\cdot\mathbf{a} \mid \varphi_\nu >$

finally resulting: $\mathbf{N}\cdot\mathbf{a} \mid \varphi_\nu > = (\nu - 1)\cdot\mathbf{a} \mid \varphi_\nu >$. (31.7)

The ket: $\mathbf{a} \mid \varphi_\nu >$ is an eigenvector of **N** with eigenvalue $\nu - 1$. I can define the new eigenvector:

$$C \mid \varphi_{\nu-1} > = \mathbf{a} \mid \varphi_\nu >$$

the equation (31.7) become: $\mathbf{N}\cdot C \mid \varphi_{\nu-1} > = (\nu - 1)\cdot C \mid \varphi_{\nu-1} >$

namely: $\mathbf{N} \mid \varphi_{\nu-1} > = (\nu - 1) \mid \varphi_{\nu-1} >$ (31.8)

With the same procedure I define the ket: $C \mid \varphi_{\nu-2} > = \mathbf{a} \mid \varphi_{\nu-1} > = \mathbf{a}\cdot\left(\mathbf{a} \mid \varphi_\nu >\right) = \mathbf{a}^2 \mid \varphi_\nu >$

and so on, finding the m^th^ eigenvector of **N** as: $\boxed{\mid \varphi_{\nu-m} > = \mathbf{a}^m \mid \varphi_\nu >}$ (31.9)

Now write the eigenvalue equation (31.1) for the ket: $\mathbf{a}^\dagger \mid \varphi_\nu >$ that is: $\mathbf{N}\cdot\mathbf{a}^\dagger \mid \varphi_\nu > = \mathbf{a}^\dagger \mid \varphi_\nu >$,

since: $\mathbf{N} = \mathbf{a}^\dagger\cdot\mathbf{a}$,

the eigenvalues equation takes the form $\mathbf{N}\cdot\mathbf{a}^\dagger \mid \varphi_\nu > = \mathbf{a}^\dagger\cdot\mathbf{a}\cdot\mathbf{a}^\dagger \mid \varphi_\nu >$ (31.10)

The product $\mathbf{a}\cdot\mathbf{a}^\dagger$ in (31.10) is equivalent to the following: $\mathbf{a}\cdot\mathbf{a}^\dagger = \mathbf{I} + \mathbf{a}^\dagger\cdot\mathbf{a}$,

therefore: $\mathbf{a}^\dagger\cdot\mathbf{a}\cdot\mathbf{a}^\dagger \mid \varphi_\nu > = \mathbf{a}^\dagger\cdot\left(\mathbf{I} + \mathbf{a}^\dagger\cdot\mathbf{a}\right) \mid \varphi_\nu > = \mathbf{a}^\dagger\cdot(\mathbf{I} + \mathbf{N}) \mid \varphi_\nu >$,

from (31.10) the equality: $\boxed{\mathbf{N}\cdot\mathbf{a}^\dagger = \mathbf{a}^\dagger\cdot(\mathbf{N} + \mathbf{I})}$. The eigenvalues equation gives: (31.11)

$$\mathbf{N}\cdot\mathbf{a}^\dagger \mid \varphi_\nu > = \mathbf{a}^\dagger\cdot(\mathbf{N} + \mathbf{I}) \mid \varphi_\nu > = \mathbf{a}^\dagger\cdot(\nu + 1) \mid \varphi_\nu > = (\nu + 1)\cdot\mathbf{a}^\dagger \mid \varphi_\nu >$$

finally resulting: $\mathbf{N}\cdot\mathbf{a}^\dagger \mid \varphi_\nu > = (\nu + 1)\cdot\mathbf{a}^\dagger \mid \varphi_\nu >$

so that $\mathbf{a}^\dagger \mid \varphi_\nu >$ is an eigenvector of **N** with eigenvalue $\nu + 1$. In that case I can define the new eigenvectors

$$\mid \varphi_{\nu+1} > = \mathbf{a}^\dagger \mid \varphi_\nu > \quad (31.12)$$

$$\mid \varphi_{\nu+2} > = \left(\mathbf{a}^\dagger\right)^2 \mid \varphi_\nu > \quad (31.13)$$

$$| \varphi_{\nu+m} > = \left(\mathbf{a}^{\dagger}\right)^{m} | \varphi_{\nu} > \qquad (31.14)$$

Resuming the previous results (31.9) and (31.14):

$$\boxed{| \varphi_{\nu-m} > = \mathbf{a}^{m} | \varphi_{\nu} >} \quad \text{eigenvalues } \nu\text{-m} \qquad (31.9')$$

$$\boxed{| \varphi_{\nu+m} > = \left(\mathbf{a}^{\dagger}\right)^{m} | \varphi_{\nu} >} \quad \text{eigenvalues } \nu\text{+m} \qquad (31.14')$$

$$| \varphi_{\nu+m} > \neq | 0 > \qquad (31.15)$$

Demonstration of |φ(λ+m)>≠|0>

Finally, results $| \varphi_{\nu+1} >$ always an eigenvector of **N** with eigenvalue ν+1. On the other hand $| \varphi_{\nu-m} >$ can be zer
In fact, calculate the average:

$$< \varphi_{\nu-m} | \mathbf{N} | \varphi_{\nu-m} > = < \varphi_{\nu-m} | (\nu - m) | \varphi_{\nu-m} > = (\nu - m) < \varphi_{\nu-m} | \varphi_{\nu-m} > \qquad (31.16)$$

this result can be rewritten as $(\nu - m) < \varphi_{\nu-m} | \varphi_{\nu-m} > = (\nu - m) \cdot \left(\| \, | \varphi_{\nu-m} > \|\right)^2$ (31.17)

$$\text{in such a way that: } \nu - m = \frac{< \varphi_{\nu-m} | \mathbf{N} | \varphi_{\nu-m} >}{\left(\| \, | \varphi_{\nu-m} > \|\right)^2} \qquad (31.18)$$

On the other hand the average of the operator **N** is:

$$< \varphi_{\nu-m} | \mathbf{N} | \varphi_{\nu-m} > = < \varphi_{\nu-m} | \mathbf{a}^{\dagger} \cdot \mathbf{a} | \varphi_{\nu-m} > = \left(\| \, \mathbf{a} | \varphi_{\nu-m} > \|\right)^2 \qquad (31.19)$$

$$\text{so that I can write as well: } \nu - m = \frac{\left(\| \, \mathbf{a} | \varphi_{\nu-m} > \|\right)^2}{\left(\| \, | \varphi_{\nu-m} > \|\right)^2} \geq 0 \qquad (31.20)$$

It follows that the sequence of eigenvectors $| \varphi_{\nu-m} >$, must terminate after a finite number of steps and there must exist one vector $| \varphi_0 >$ such that $\boxed{\mathbf{a} | \varphi_0 > = | 0 >}$.

Normalization:

define the normalized eigenvector as $| \phi_0 > = \dfrac{| \varphi_0 >}{\| \, | \varphi_0 > \|} = C_0 | \phi_0 >$ $\qquad C_0 = 1$ (31.21)

Various cases

$$\text{generalizing I get: } | \phi_n > = \frac{| \varphi_n >}{\| \, | \varphi_n > \|} = C_n \cdot \left(\mathbf{a}^{\dagger}\right)^n | \phi_0 > \qquad (31.22)$$

$$\boxed{| \phi_n > = C_n \cdot \left(\mathbf{a}^{\dagger}\right)^n | \phi_0 >} \qquad (31.23)$$

$$C_n = \frac{1}{k_n}$$

I'm looking for a relation between C_n and C_{n-1}. Consider therefore the normalization of the eigenvalue equation wit
$\nu = n$:

$$\frac{\mathbf{N} | \varphi_n >}{\| \, | \varphi_n > \|} = \frac{n | \varphi_n >}{\| \, | \varphi_n > \|} \qquad (31.24)$$

thanks to (31.22) eq. (31.24) it can be rewritten:

$$\mathbf{N} \mid \phi_n > = n \mid \phi_n > \tag{31.25}$$

whose norm is: $\| \mid \phi_n > \| = \sqrt{< \phi_n \mid \phi_n >} = 1$ (31.26)

Now calculate the square of (31.26) and substitute in it eq.(31.23):

$$\left(\| \mid \phi_n > \|\right)^2 = \left[\| C_n \cdot \left(\mathbf{a}^\dagger\right)^n \mid \phi_0 > \|\right]^2 = \left(|C_n|\right)^2 \cdot < \phi_0 \mid \left(\mathbf{a} \cdot \mathbf{a}^\dagger\right)^n \mid \phi_0 > = 1 \tag{31.27}$$

Calculation of || |φ>||²

$$\| C_n \cdot \left(\mathbf{a}^\dagger\right)^n \mid \phi_0 > \| = \left[C_n \cdot \left(\mathbf{a}^\dagger\right)^n \mid \phi_0 >\right]^\dagger C_n \cdot \left(\mathbf{a}^\dagger\right)^n \mid \phi_0 > = < \phi_0 \mid (C_n *) \cdot \left[\left(\mathbf{a}^\dagger\right)^\dagger\right]^n \cdot C_n \cdot \left(\mathbf{a}^\dagger\right)^n \mid \phi_0 >$$

$$\left[\left(\mathbf{a}^\dagger\right)^\dagger\right]^n \cdot \left(\mathbf{a}^\dagger\right)^n = (\mathbf{a})^n \cdot \left(\mathbf{a}^\dagger\right)^n = \left(\mathbf{a} \cdot \mathbf{a}^\dagger\right)^n$$

$$< \phi_0 \mid (C_n *) \cdot \left[\left(\mathbf{a}^\dagger\right)^\dagger\right]^n \cdot C_n \cdot \left(\mathbf{a}^\dagger\right)^n \mid \phi_0 > = < \phi_0 \mid (C_n *) \cdot \mathbf{a}^n \cdot C_n \cdot \left(\mathbf{a}^\dagger\right)^n \mid \phi_0 >$$

$$< \phi_0 \mid C_n * \cdot \mathbf{a}^n \cdot C_n \cdot \left(\mathbf{a}^\dagger\right)^n \mid \phi_0 > = C_n * \cdot C_n < \phi_0 \mid \left(\mathbf{a} \cdot \mathbf{a}^\dagger\right)^n \mid \phi_0 > = \left(|C_n|\right)^2 < \phi_0 \mid \left(\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}\right)^n \mid \phi_0 >$$

Calculation of || |φ>||²

In the average (31.27) there is the previously defined ket (31.23):

$$\left(\mathbf{a}^\dagger\right)^n \mid \phi_0 > = \frac{1}{C_n} \mid \phi_n > = \frac{\mathbf{a}^\dagger \mid \phi_{n-1} >}{C_{n-1}} \tag{31.28}$$

which substituted in the result (31.27), gives:

$$< \phi_0 \mid \left(\mathbf{a} \cdot \mathbf{a}^\dagger\right)^n \mid \phi_0 > = \frac{1}{\left(|C_n|\right)^2} = \frac{< \phi_{n-1} \mid \mathbf{a} \cdot \mathbf{a}^\dagger \mid \phi_{n-1} >}{\left(|C_{n-1}|\right)^2} = \frac{< \phi_{n-1} \mid \left(\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}\right) \mid \phi_{n-1} >}{\left(|C_{n-1}|\right)^2}$$

$$\left(|C_n|\right)^2 \cdot \left[< \phi_0 \mid \left(\mathbf{a} \cdot \mathbf{a}^\dagger\right)^n \mid \phi_0 >\right]^2 = \left(|C_n|\right)^2 \cdot \left(< \phi_n \mid \phi_n >\right)^2 = \left(|C_n|\right)^2 = 1$$

$$\frac{1}{\left(|C_n|\right)^2} = n \cdot \frac{< \phi_{n-1} \mid \phi_{n-1} >}{\left(|C_{n-1}|\right)^2} = \frac{n}{\left(|C_{n-1}|\right)^2} \qquad < \phi_{n-1} \mid \phi_{n-1} > = 1$$

$$\frac{< \phi_{n-1} \mid \left(\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}\right) \mid \phi_{n-1} >}{\left(|C_{n-1}|\right)^2} = \frac{< \phi_{n-1} \mid (\mathbf{N} + 1) \mid \phi_{n-1} >}{\left(|C_{n-1}|\right)^2} = n \cdot \frac{< \phi_{n-1} \mid \phi_{n-1} >}{\left(|C_{n-1}|\right)^2}$$

<n|

Sequence

$$\boxed{C_n = \frac{1}{\sqrt{n!}}} \tag{31.29}$$

The sought eigenvector is: $\boxed{\mid \phi_n > = \frac{1}{\sqrt{n!}} \cdot \left(\mathbf{a}^\dagger\right)^n \mid \phi_0 >}$ with eigenvalue n, (31.30)

(that is the solution of the eigenvalues equation: $\mathbf{N} \mid \phi_n > = n \mid \phi_n >$.)

They are orthonormal $< \phi_n | \phi_\nu > = \delta_{n,\nu}$ 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.

$$C | \phi_{\nu-1} > = \mathbf{a} | \phi_\nu >$$

$$< \phi_{\nu-1} | C^* \cdot C | \phi_{\nu-1} > = < \phi_\nu | \mathbf{a}^\dagger \cdot \mathbf{a} | \phi_\nu > = < \phi_\nu | \mathbf{N} | \phi_\nu > = n < \phi_\nu | \phi_\nu >$$

$$(|C|)^2 < \phi_{\nu-1} | \phi_{\nu-1} > = n < \phi_\nu | \phi_\nu > \qquad < \phi_{\nu-1} | \phi_{\nu-1} > = 1 \qquad < \phi_\nu | \phi_\nu > = 1$$

$$C = \sqrt{n}$$

$$C_1 | \phi_{\nu-1} > = \mathbf{a}^\dagger | \phi_\nu >$$

$$< \phi_{\nu-1} | C_1^* \cdot C_1 | \phi_{\nu-1} > = < \phi_\nu | \mathbf{a} \cdot \mathbf{a}^\dagger | \phi_\nu >$$

$$\mathbf{a} \cdot \mathbf{a}^\dagger = \mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}$$

$$< \phi_{\nu-1} | C_1^* \cdot C_1 | \phi_{\nu-1} > = < \phi_\nu | \mathbf{a} \cdot \mathbf{a}^\dagger | \phi_\nu > = < \phi_\nu | \left(\mathbf{I} + \mathbf{a}^\dagger \cdot \mathbf{a}\right) | \phi_\nu > = n < \phi_\nu | \phi_\nu >$$

$$\left(|C_1|\right)^2 < \phi_{\nu-1} | \phi_{\nu-1} > = < \phi_\nu | (\mathbf{I} + \mathbf{N}) | \phi_\nu > = (n+1) < \phi_\nu | \phi_\nu >$$

$$|C_1| = \sqrt{n+1}$$

(***Ladder operators***) $\boxed{\mathbf{a} | \phi_n > = \sqrt{n} | \phi_{n-1} >}$ annihilation operator (31.31)

$\boxed{\mathbf{a}^\dagger | \phi_n > = \sqrt{n+1} | \phi_{n+1} >}$ creation operator (31.32)

Consider the set of all vectors $| \Psi > = \sum_{n=0}^{\infty} \left(\alpha_n | \phi_n >\right)$ where the α_n are complex numbers and

$$\sum_{n=0}^{\infty} \left[\left(|\alpha_n|\right)^2\right] < \infty$$

It forms a linear space, that is the Hilbert space $\mathbb{H}$ spanned by $| \phi_n >$

The space of all $| \Psi >$ for which $\sum_{n=0}^{\infty} \left[\left(|\alpha_n|\right)^2 \cdot (n+1)^p\right] < \infty \qquad p = 0, 1, 2, 3 .. \infty$

will be denoted by Σ (Schwartz space) $\Sigma \subset \mathbb{H}$.

All the operators representing observables can be defined on the whole space Σ but not on all $\mathbb{H}$.

All observables are functions of the operators $\mathbf{a}$ and $\mathbf{a}^\dagger$ given by (31.31) and (31.32) known for all $| \Psi >$.

Calculation of the diagonal matrix elements:

$$\mathbf{H} = \hbar \cdot \omega \cdot \mathbf{H_0} = \hbar \cdot \omega \cdot \left(\mathbf{N} + \frac{1}{2} \cdot \mathbf{I}\right) \qquad \mathbf{N} | \varphi_\nu > = \nu | \varphi_\nu >$$

$$\mathbf{H} | \phi_n > = \hbar \cdot \omega \cdot \left(\mathbf{N} + \frac{1}{2} \cdot \mathbf{I}\right) | \phi_n > = \hbar \cdot \omega \cdot \left(\nu + \frac{1}{2}\right) | \phi_n >$$

$$< \phi_\nu \mid \mathbf{H} \mid \phi_\nu > = \hbar\cdot\omega < \phi_\nu \mid \left(\mathbf{N} + \frac{1}{2}\cdot\mathbf{I}\right) \mid \phi_\nu > = \hbar\cdot\omega\cdot\left(\nu + \frac{1}{2}\right) < \phi_\nu \mid \phi_\nu > = \hbar\cdot\omega\cdot\left(\nu + \frac{1}{2}\right)\cdot\left(\left|\mid \varphi_\nu >\right|\right)^2$$

$$\boxed{E_\nu = < \phi_\nu \mid \mathbf{H} \mid \phi_\nu > = \hbar\cdot\omega\cdot\left(\nu + \frac{1}{2}\right)} \qquad \left(\left|\mid \varphi_\nu >\right|\right)^2 = 1 \qquad (31.33)$$

$$E_\nu = \Delta E\cdot\left(\nu + \frac{1}{2}\right) \qquad \Delta E = \hbar\cdot\omega$$

the diagonal matrix elements are the possible energy values of the QM oscillator. One can excite the harmonic oscillat into any one of a discrete number of ***states*** described by $\mid \phi_\nu >$, the system is in a mixture of states. The mixture can described by the set of vectors $\mid \phi_0 >$, $\mid \phi_1 >$, $\mid \phi_2 >$,..., $\mid \phi_\nu >$ and a set of relative probabilities w_0, w_1, w_2,...,w_n,...proportional to the height of the bump corresponding to the energy E_n .

$$\sum_n w_n = 1$$

In a collection of N elemets (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 $\mid \phi_0 >$, (See Frank & Hertz experiment) . If there is only one state $\mid \phi_{n0} >$ then the quantum system is in a ***pure state*** $\mid \phi_{n0} >$ and the corresponding energy is the only one E_{n0} .

II axiom. A physical QM system characterized by a projection operator **P** on a one-dimensional subspace $P\mathbb{H}$ is in a pure state.

Books

Books

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[4] Albert Messiah - ***Quantum Mechanics*** - Vol. I&II North - Holland Publishing company

[5] Kenneth R. Lang - ***Astrophysical Formulae*** - Second ed. Springer - Verlag

[6] Arno Bhöm - ***Quantum Mechanics*** - Springer - Verlag

[7] Gianfranco Pradisi - ***Lezioni di metodi matematici della fisica*** - Edizioni Della Normale

[8] Fritz Reinhardt, Heinrich Soeder - ***Atlante di Matematica*** - Editore Ulrico Hoepli Milano

Books