

# **An introduction to Schrödinger quantum mechanics**

**Suitable for people interested in its philosophical implications**

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## Contents

1. Introduction.....	<u>1</u>
Abstract.....	<u>1</u>
Features of Schrödinger quantum mechanics.....	<u>1</u>
2. Mathematical elements.....	<u>3</u>
Complex numbers.....	<u>3</u>
Geometrical representation of complex numbers.....	<u>3</u>
Examples of geometrical representation of complex numbers.....	<u>4</u>
Complex functions of real variables.....	<u>5</u>
Derivative of a complex function.....	<u>5</u>
Partial derivatives.....	<u>6</u>
3. Schrödinger equations.....	<u>9</u>
State description in classical mechanics.....	<u>9</u>
Quantum operators.....	<u>9</u>
First Schrödinger equation.....	<u>10</u>
Simplifying first Schrödinger equation.....	<u>11</u>
Bohr energy levels.....	<u>11</u>
State description in quantum mechanics.....	<u>13</u>
Second Schrödinger equation.....	<u>13</u>
A brief recapitulation.....	<u>13</u>
4. Applications.....	<u>15</u>
Tunnel effect.....	<u>15</u>
Transmission coefficient.....	<u>16</u>
Alpha radioactivity.....	<u>17</u>
5. Heisenberg indeterminacy principle.....	<u>19</u>
Commutative operators.....	<u>19</u>
Non commutative operators.....	<u>19</u>
The effect of measurement on $\Psi$ function.....	<u>20</u>
Mean values.....	<u>21</u>
Applications of the indeterminacy principle.....	<u>22</u>
6. Links and further reading.....	<u>25</u>
Physics.....	<u>25</u>
Philosophy.....	<u>25</u>
Further reading.....	<u>25</u>
Appendix.....	<u>27</u>
Linear differential equations.....	<u>27</u>



## 1. Introduction.

The main goal of this article is to provide a mathematical introduction to Schrödinger quantum mechanics suitable for people interested in its philosophical implications.

### Abstract.

A brief explanation of [complex functions](#), including [derivatives](#) and [partial derivatives](#), is given. [First](#) and [second](#) Schrödinger equations are formulated and some of their physical consequences are analysed, particularly the derivation of Bohr [energy levels](#), the forecast of the [tunnel effect](#) and an explanation of [alpha radioactivity](#). These examples are chosen in order to show real physical applications of Schrödinger equations. The exposition of Heisenberg [indeterminacy principle](#) begins with an analysis of the properties of [commutative](#) and [non commutative](#) operators, continues with a brief explanation of [mean values](#) and ends with some physical [applications](#).

Schrödinger quantum theory is formulated in an axiomatic fashion. No historical analysis is developed to justify the formulation of the two Schrödinger equation: Their only justification derives from their success in explaining physical facts. The philosophical background I use in this article is due to [logical positivism](#) and its analysis of the [structure](#) of a scientific theory. In this perspective, Schrödinger equations are the theoretical axioms of the theory; the probabilistic interpretation of Schrödinger equations plays the roles of the rules of correspondence, establishing a correlation between real objects and the abstract concepts of the theory; the observational part of the theory describes observation about radioactivity, spectral wavelengths and similar events.

### Features of Schrödinger quantum mechanics.

Schrödinger quantum mechanics is a restricted portion of quantum theory. Its main limitation is due to the fact that it is a non-relativistic theory. This is a very important limitation, because every fundamental theory must be a relativistic one. Schrödinger equations find an application only in situation in which the energy is small. Events concerning creation or annihilation of particles require a great value of the energy, and thus this type of events is out of the scope of Schrödinger quantum theory.

However, this theory gives an explanation of important facts, like the quantization of the energy levels in hydrogen atom. The indeterminacy principle is derivable from Schrödinger quantum mechanics, and this fact is of a primary interest from a philosophical analysis.

Perhaps the most important point concerning Schrödinger quantum mechanics is that its mathematical complexity is not overwhelming. A philosophical analysis of a scientific theory requires an effective comprehension of the theory, which is often very difficult due to the complexity of the required mathematical background. Schrödinger quantum mechanics requires a mathematical knowledge limited to the the first-year calculus: derivative and integral of a real function. With a little effort, derivative, integral and expansion of complex functions can be understood using the analogy with real functions.



## 2. Mathematical elements.

Some mathematical instruments necessary for a comprehension of quantum mechanics are described: complex numbers, [complex functions](#), [derivatives](#) and [partial derivatives](#) of complex functions.

### Complex numbers.

A complex number is a number of the type  $a+ib$  where  $a$  and  $b$  are real numbers, called respectively the real and the imaginary part, and  $i^2 = -1$ . If  $b=0$  then the complex number is also a real number, that is a real number is a complex number which has no imaginary part.

Let  $z=a+ib$  be a complex number; from  $z$  others mathematical entities are defined:

- The complex conjugate of  $z$  is the complex number  $a-ib$  and is denoted by  $z^*$ . If  $z$  is a real number then  $z=z^*$ . Note that  $z \cdot z^* = a^2 + b^2$  is a real number.
- The module (also called absolute value) of  $z$  is the real number  $\sqrt{a^2 + b^2}$ ; it is denoted by  $|z|$ . Between the module and the complex conjugate holds the relation  $|z|^2 = z \cdot z^*$ .
- The square of  $z$  is the complex number  $z \cdot z = a^2 - b^2 + 2abi$  and is denoted by  $z^2$ . In general,  $z^2 \neq |z|^2$ . Only if  $z$  is a real number then  $z^2 = |z|^2$ .

The four basic operation (addition, subtraction, multiplication and division) between complex numbers are carried out like the corresponding operations on real polynomials, remembering that  $i^2 = -1$ . Some examples:

- $(3+5i)(2-3i) = 6-9i+10i-15i^2 = 6+i+15 = 21+i$
- $(3-4i)+(6+i) = 3-4i+6+i = 9-3i$
- $(3-4i)-(6+i) = 3-4i-6-i = -3-5i$

### Geometrical representation of complex numbers.

Complex numbers can be geometrically represented on the two dimensional Cartesian coordinate system, assigning the real part to the  $x$ -axis and the imaginary part to the  $y$ -axis. The complex number  $z=a+ib$  is represented as the vector from the origin to the point  $(a,b)$ . In this geometrical interpretation of complex numbers some operations have an intuitive meaning.

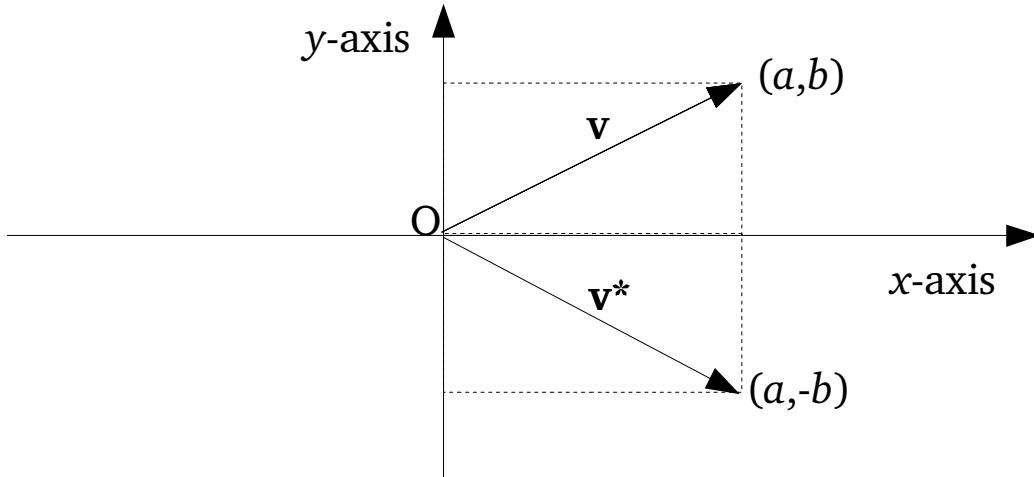
- The module of a complex number is the length of the vector representing the complex number.
- The addition of two complex numbers is the analogous of the sum of the corresponding vectors.
- The multiplication of a real number and a complex number is the analogous of multiplying the vector corresponding to the complex number by a scalar.

The following formula, known as Euler's formula, defines an interesting relation between complex numbers and trigonometric functions:  $e^{ix} = \cos x + i \sin x$ .

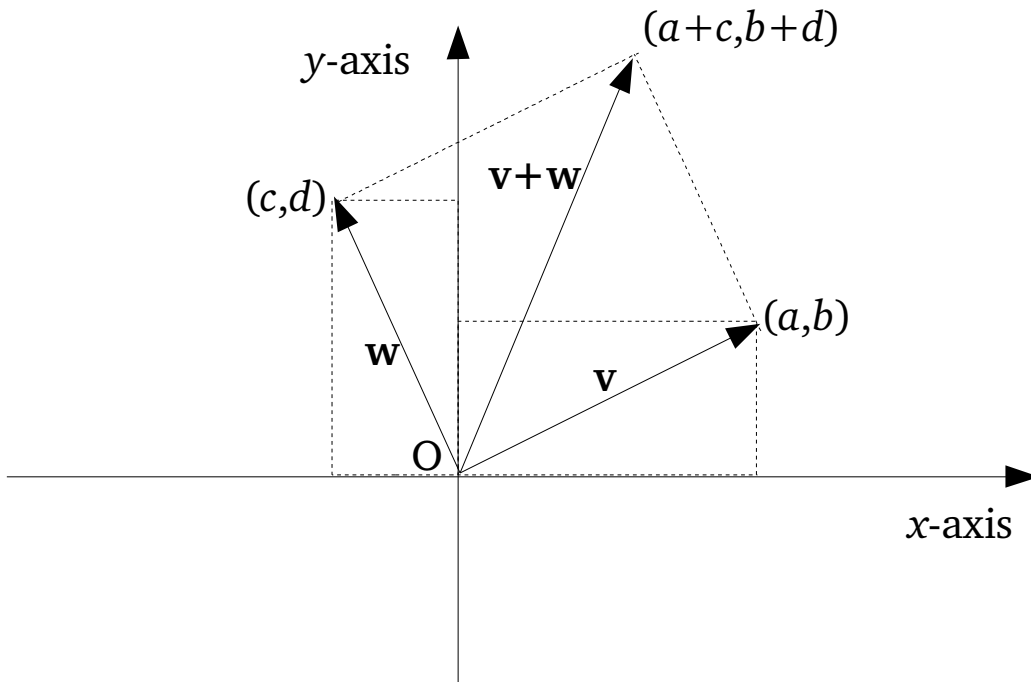
**Examples of geometrical representation of complex numbers.**

Vector  $\mathbf{v}$  represents the complex number  $a+ib$

Vector  $\mathbf{v}^*$  represents the complex conjugate of  $a+ib$



The sum of complex number  $v=a+ib$  and  $w=c+id$  is interpreted as the sum of the corresponding vectors  $\mathbf{v}$  and  $\mathbf{w}$





**Complex functions of real variables.**

Let  $X$  and  $Y$  be two sets and let  $f$  be a rule that assigns to every element of  $X$  exactly one element of  $Y$ ;  $f$  is called a function from  $X$  to  $Y$  and the sets  $X$  and  $Y$  are called respectively the domain and the co-domain (or range) of the function  $f$ . A function  $f$  from  $X$  to  $Y$  is represented by the notation  $y = f(x)$  where  $y$  is the element of  $Y$  assigned to the element  $x$  of  $X$ . The element  $x$  is called the argument of the function  $f$  and the element  $y$  is called the value of  $f$  for the argument  $x$ . The elements  $x$  and  $y$  are also called variables;  $x$  is the independent variable and  $y$  is the dependent variable.

If the domain and the co-domain of a function  $f$  are equal to the set  $R$  of real numbers (that is:  $X=Y=R$ ) then the function  $f$  is called a real function of a real variable. A well known function of this kind is the function square ( $y = x^2$ ) which associates to every real number  $x$  its square  $x^2$ .

Multiplication between two real numbers is a real function of two real variables; it is an example of functions of the type  $y = f(x_1, x_2)$  where  $x_1$  and  $x_2$  are real numbers. From a formal point of view, a function like  $y = f(x_1, x_2)$  with  $x_1$  and  $x_2$  real numbers is a function from  $R \times R$  to  $R$ , where  $R \times R$  is the Cartesian product of  $R$  by itself: The domain of  $f$  is the set of all ordered pairs of real numbers, that is the set whose elements are the ordered pairs  $\langle a, b \rangle$  for every real number  $a$  and  $b$ .

Complex functions of a real variable are functions from the set  $R$  of real number to the set  $C$  of complex numbers; a function of this kind associates to every real number exactly one complex number. An example is the square root function that assign to every real number its square root: If the argument of this function is less than zero, then the value of the function is a complex number.

A complex function of  $n$  real variables is a function whose arguments are  $n$  real numbers and whose value is a complex number. It is a function from  $R^n$  to  $C$ .

From this point, Greek letters will be used to denote complex functions or complex numbers; Latin letters will be used to denote real functions or real numbers. Here are some examples:

- $\varphi(x)$  and  $\Psi(x)$  denote complex functions of a real variable.
- $\varphi(x, y)$  and  $\Psi(x, y, z)$  denote complex functions of real variables (two and three real variables, respectively).
- $\varphi$  and  $\Psi$  denote complex functions of a real variables, without specifying the number of real variables.
- $\sigma$  denotes a complex number.
- $x y z$  denote real numbers.

**Derivative of a complex function.**

The derivative of a function is the rate of change of the value of the function with respect to its argument. There is no substantial difference between the derivative of a real function and the derivative of a complex function, so it is possible to use the usual rules applicable to the

derivative of a real function. There are some notations to denote the derivative of a function  $\varphi(x)$ ; the most common are  $\varphi'(x)$ ,  $d\varphi(x)/dx$ ,  $D\varphi(x)$ . Here is a small table with the derivative of some functions.

Function	Derivative	Notes
$\varphi(x) = x^n$	$\varphi'(x) = n x^{n-1}$	$n$ is a natural number
$\varphi(x) = \sin(x)$	$\varphi'(x) = \cos(x)$	
$\varphi(x) = \cos(x)$	$\varphi'(x) = -\sin(x)$	
$\varphi(x) = e^x$	$\varphi'(x) = e^x$	$e$ is the base of natural logarithms ( $e=2.718\dots$ )
$\varphi(x) = e^{-x}$	$\varphi'(x) = -e^{-x}$	
$\varphi(x) = e^{kx}$	$\varphi'(x) = k e^{kx}$	
$\varphi(x) = e^{ix}$	$\varphi'(x) = e^{i(x+\pi/2)}$	
$\varphi(x) = e^{-ix}$	$\varphi'(x) = -e^{-i(2x+\pi)/2}$	
$\varphi(x) = e^{kix}$	$\varphi'(x) = k e^{i(kx+\pi/2)}$	
$\varphi(x) = \ln(x)$	$\varphi'(x) = 1/x$	$\ln$ is the natural logarithm

Let  $\varphi(x)$  and  $\Psi(x)$  be two complex functions of a real variable. The derivatives of their addition, multiplication and division are:

$$\begin{aligned} D(\varphi(x) + \Psi(x)) &= \varphi'(x) + \Psi'(x) \\ D(\varphi(x) \cdot \Psi(x)) &= \varphi(x) \cdot \Psi'(x) + \varphi'(x) \cdot \Psi(x) \\ D(\varphi(x) / \Psi(x)) &= \varphi'(x) / \Psi(x) - \Psi'(x) \cdot \varphi(x) / (\Psi(x))^2 \end{aligned}$$

The derivative  $\varphi'(x)$  of a function  $\varphi(x)$  is a function too; thus there exists also the derivative of  $\varphi'(x)$ , which is called the second derivative of  $\varphi(x)$  and is usually denoted by one of the following expressions:  $\varphi''(x)$ ,  $d^2\varphi(x)/dx^2$ .

### Partial derivatives.

Let  $\varphi(x, y)$  be a complex function of two real variables. As an example, let  $\varphi(x, y) = e^{ixy}$ . There are two different rates of change of this function, one with respect to the  $x$  variable, the other with respect to the  $y$  variable. The first rate of change is determined considering the  $y$  variable as a constant and calculating the usual derivative of  $\varphi$ . This is called the first partial derivative of  $\varphi(x, y)$  with respect to  $x$  and is denoted by  $\partial\varphi(x, y) / \partial x$ . In the example we have  $\partial\varphi(x, y) / \partial x = \partial e^{ixy} / \partial x = y e^{i(xy + \pi/2)}$ .

There exists also the first partial derivative of  $\varphi(x, y)$  with respect to  $y$ , calculated assuming  $x$  constant, and denoted by  $\partial\varphi(x, y) / \partial y$ . Continuing the example:

$$\partial\varphi(x, y) / \partial y = \partial e^{ixy} / \partial y = x e^{i(xy + \pi/2)}.$$

The second partial derivatives of  $\varphi(x, y)$  with respect to  $x$  and  $y$  is the first partial derivative of  $\partial\varphi(x, y) / \partial x$  with respect to  $y$ . It is denoted by  $\partial^2\varphi(x, y) / \partial x \partial y$  and is calculated in the following way:

1. Consider  $y$  as a constant and determine the derivative of  $\varphi(x, y)$  with respect to  $x$ .
2. Consider  $x$  as a constant in the derivative and calculate another derivative with respect to  $y$ .

A simple example: let  $z = x^3 y$ . We have:

- $\partial z / \partial x = 3 x^2 y$
- $\partial^2 z / \partial x \partial y = 3 x^2$
- $\partial z / \partial y = x^3$
- $\partial^2 z / \partial y \partial x = 3 x^2$

Note that, in the example,  $\partial^2 z / \partial x \partial y = \partial^2 z / \partial y \partial x$ . In this article are mainly used function satisfying this relation, although it does not hold in general.



### 3. Schrödinger equations.

A brief presentation of the state description in classical physics precedes the analysis of the rules that associate a [quantum operator](#) to a classical physical quantity; then the [first](#) Schrödinger equation is introduced and, as an example of application of the equation, the formula for Bohr [energy levels](#) is derived. The section ends with an introduction to the [state description](#) in quantum mechanics and the role of the [second](#) Schrödinger equation.

#### State description in classical mechanics.

Consider a classical particle (that is a particle moving according to Newton's laws of motion), with a given mass  $m$ , that is subjected to a field of force. Suppose that:

- the position and the momentum of that particle at a given time  $t_0$  are known
- the mathematical expression of the field acting on the particle is known.

Then, according to classical physics, it is possible to determine:

- the position and the momentum of the particle at every time  $t$
- every other mechanical quantity at every time  $t$ .

If the initial position and momentum of a particle are known, with the exact expression of the forces acting on that particle, then the position and the momentum of the particle can be calculated at every time in the future and in the past. Since every classical mechanical quantity is uniquely defined by means of position and momentum, which are known at every time, then also the value of every classical mechanical quantity at every time is known.

In classical physics, the position of a particle with respect to a given frame of reference is expressed by means of a vector  $\mathbf{q}$  or by means of the three components  $q_1, q_2, q_3$  of this vector.

The momentum of a particle is expressed by the vector  $\mathbf{p}=m\mathbf{v}$ , where  $\mathbf{v}$  is the velocity of the particle with respect to the given frame of reference. The three components of the vector  $\mathbf{p}$  are denoted  $p_1, p_2, p_3$ .

The mechanical energy  $E$  of the particle is given by the sum of kinetic energy  $T$  and potential energy  $U$ . The following relations hold:

- (3.1)  $E = T + U$
- (3.2)  $T = \frac{1}{2} m v^2 = \frac{1}{2} \mathbf{p}^2/m = (p_1^2 + p_2^2 + p_3^2) / (2m)$
- (3.3)  $E = (p_1^2 + p_2^2 + p_3^2) / (2m) + U$

Relations (3.1)-(3.3), derived in a simple classical system, are nevertheless useful in quantum mechanics.

#### Quantum operators.

An operator is a rule that transcripts (that is transforms) a given function in another function. Quantum mechanics makes use of operator for translating classical mechanical equations in quantum mechanical equations.

Let  $u$  be a classical mechanical quantity. Every classical mechanical quantity is defined by position and momentum, so  $u$  is a function of  $\mathbf{q}$  and  $\mathbf{p}$ :  $u = u(q_1, q_2, q_3, p_1, p_2, p_3)$

In quantum mechanics, an operator  $u_{op}$  corresponding to  $u$  is defined by means of the following two rules acting on the equation  $u = u(q_1, q_2, q_3, p_1, p_2, p_3)$ .

1. Substitute every occurrences of  $q_k$  with the operator "multiplication by  $q_k$ " and every occurrences of  $f(q_k)$  with the operator "multiplication by  $f(q_k)$ ".
2. Substitute every occurrences of  $p_k^n$  with the operator  $\left(\frac{\hbar}{2\pi i}\right)^n \frac{\partial^n}{\partial q_k^n}$ .

For example, let  $u$  be the mechanical energy  $E$  given by (3.3). The operator  $E_{op}$  associated to  $E$  is:

$$(3.4) \quad E_{op} = \frac{1}{2m} \left(\frac{\hbar}{2\pi i}\right)^2 \left(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2} + \frac{\partial^2}{\partial q_3^2}\right) + U(q_1, q_2, q_3).$$

Note that in (3.4) the expression  $U(q_1, q_2, q_3)$  means "multiply by  $U(q_1, q_2, q_3)$ ".

### First Schrödinger equation.

Let  $u$  be a given classical mechanical quantity; let  $u_{op}$  the quantum operator associated to  $u$ ; the first Schrödinger equation for  $u$  is

$$(3.5) \quad u_{op} \varphi(\mathbf{q}) = u \cdot \varphi(\mathbf{q}).$$

For example, if  $u = E$  then the first Schrödinger equation for the energy  $E$  is

$$(3.6) \quad \frac{1}{2m} \left(\frac{\hbar}{2\pi i}\right)^2 \left(\frac{\partial^2 \varphi(\mathbf{q})}{\partial q_1^2} + \frac{\partial^2 \varphi(\mathbf{q})}{\partial q_2^2} + \frac{\partial^2 \varphi(\mathbf{q})}{\partial q_3^2}\right) + U(q_1, q_2, q_3) \cdot \varphi(\mathbf{q}) = E \cdot \varphi(\mathbf{q}).$$

In the first Schrödinger equation the complex function  $\varphi(\mathbf{q})$  is the unknown and  $u$  is a parameter. For every value of  $u$  there is a complex function  $\varphi(\mathbf{q})$  that is a solution of the equation. However, not every  $\varphi(\mathbf{q})$  is acceptable from a physical point of view, so some restrictions are imposed on  $\varphi(\mathbf{q})$ . One of such restrictions is the requirement that the quadratic integral of  $\varphi(\mathbf{q})$  exists and is finite, that is  $\varphi(\mathbf{q})$  is acceptable as a solution only if the integral  $\int |\varphi(\mathbf{q})|^2 dx$ , extended over the domain to which  $x$  belongs, is finite. Another requirement is that  $\varphi(\mathbf{q})$  must be finite for all values of its argument  $\mathbf{q}$ .

With such requirements, not for every value of  $u$  has the equation an acceptable solution  $\varphi(\mathbf{q})$ . The physical meaning of first Schrödinger equation is precisely that only for certain values of  $u$  the equation has a solution  $\varphi(\mathbf{q})$ : those values are the admissible values for the physical quantity  $u$ . Consider the equation (3.6) (first Schrödinger equation for energy  $E$ ): it

admits solutions, compatible with the requirements on  $\varphi(\mathbf{q})$ , only for a discrete set of values of  $E$ , not for every value of  $E$ . Equation (3.6) thus determines the admissible value for mechanical energy: they are the values giving a solution to the equation. While in classical physics every value for the energy  $E$  is admissible, in quantum mechanics only those values of the energy that satisfies the first Schrödinger equation are admissible: this is the root of the quantization of the energy levels.

A brief recapitulation. Let  $u$  be a physical quantity; every value of  $u$  is acceptable in classical physics. In quantum mechanics an operator  $u_{op}$  is defined according to certain rules, so to construct the equation  $u_{op}\varphi(\mathbf{q}) = u \cdot \varphi(\mathbf{q})$ . Some conditions of regularity are imposed on  $\varphi(\mathbf{q})$ . The equation has solutions only for certain values of  $u$ : those are the only acceptable values of  $u$ . The physical quantity  $u$  has been quantized.

The values  $u_i$  for which the first Schrödinger equation  $u_{op}\varphi(\mathbf{q}) = u \cdot \varphi(\mathbf{q})$  has admissible solutions are called *eigenvalues* and the corresponding solutions  $\varphi_i(\mathbf{q})$  are called *eigenfunctions*. This words derives from the German terms *eigenwert* and *eigenfunktion*, utilized by Schrödinger in his four articles entitled *Quantisierung als Eigenwertproblem* (1926).

### Simplifying first Schrödinger equation.

With few mathematical passages and using the constant  $\hbar = \frac{h}{(2\pi)}$  the first Schrödinger equation for the energy  $E$  becomes

$$\left( \frac{\partial^2 \varphi(\mathbf{q})}{\partial \mathbf{q}_1^2} + \frac{\partial^2 \varphi(\mathbf{q})}{\partial \mathbf{q}_2^2} + \frac{\partial^2 \varphi(\mathbf{q})}{\partial \mathbf{q}_3^2} \right) + \frac{2m}{\hbar^2} [E - U(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)] \cdot \varphi(\mathbf{q}) = 0 .$$

The equation can be simplified with the introduction of the Laplace operator  $\nabla^2$  as an abbreviation for  $\left( \frac{\partial^2}{\partial \mathbf{q}_1^2} + \frac{\partial^2}{\partial \mathbf{q}_2^2} + \frac{\partial^2}{\partial \mathbf{q}_3^2} \right)$  (the symbol  $\nabla$  is called the *nabla* operator). The first Schrödinger equation for the energy  $E$  can be written in the compact form:

$$(3.7) \quad \nabla^2 \varphi(\mathbf{q}) + \frac{2m}{\hbar^2} [E - U(\mathbf{q})] \cdot \varphi(\mathbf{q}) = 0 .$$

### Bohr energy levels.

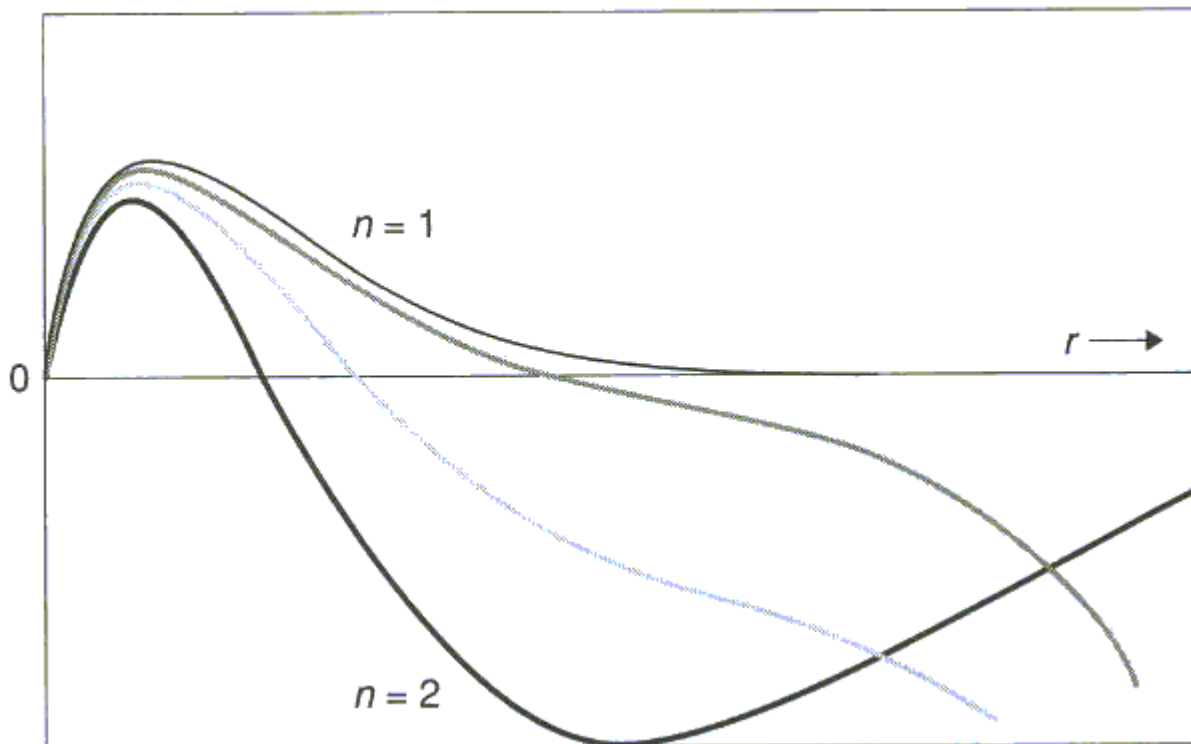
In Bohr theory of the hydrogen atom, the angular momentum of the electron in its orbit is a multiple of the quantity  $h/2\pi$ , so the energy of the electron is quantized. The values  $E_n$  of the energy of the electron, called the energy levels, are given by the formula

$$(3.8) \quad E_n = -\frac{1}{n^2} \frac{me^4}{2\hbar^2}.$$

This formula is derivable from the first Schrödinger equation. Consider an application of the equation (3.7) to the hydrogen atom: The expression for the potential  $U$  is  $U = -e^2/r$  where  $e$  is the electron charge and  $r$  is the distance from the electron. In polar coordinates the equation (3.7) became

$$(3.9) \quad \frac{d^2 \Omega(r)}{dr^2} + \frac{2}{r} \frac{d\Omega(r)}{dr} + \frac{2m}{\hbar^2} \left[ E + \frac{e^2}{r} \right] \Omega(r) = 0$$

where  $\Omega(r)$  is a function of the distance  $r$ . The eigenvalues of the equation (3.9) are the values of  $E$  given by equation (3.8). Thus the first Schrödinger equation gives a correct deduction of the energy levels of Bohr theory. Values of  $E$  different from series (3.8) generate solutions  $\Omega(r)$  not acceptable. The figure shows the diagram of four solutions, two acceptable and two not acceptable.



Labels  $n=1$  and  $n=2$  indicate the functions  $r\cdot\Omega(r)$  corresponding to eigenvalues  $E_1$  and  $E_2$ . These functions satisfy the restrictions imposed on the solutions of the first Schrödinger equation. The others two divergent functions, corresponding to values of  $E$  between  $E_1$  and  $E_2$ , do not satisfy these restrictions.

Source: Wick, Giancarlo, "Meccanica quantistica", *Enciclopedia delle scienze fisiche*, Treccani, 1993.



**State description in quantum mechanics.**

The state  $S$  of a quantum system is completely described by a complex function  $\Psi(\mathbf{q})$  depending from position  $\mathbf{q}$ .

Let  $u$  be a classical physical quantity and let  $u_{op}$  be the corresponding quantum operator. The first Schrödinger equation is  $u_{op}\varphi(\mathbf{q})=u\cdot\varphi(\mathbf{q})$ . The eigenvalues  $u_i$  are the admissible values of  $u$ .

The complex function  $\Psi(\mathbf{q})$  can be represented as a sum of the eigenfunctions:

$$(3.10) \quad \Psi(\mathbf{q}) = \sum_{i=1}^{i=\infty} \sigma_i \cdot \varphi_i(\mathbf{q})$$

Complex numbers  $\sigma_i$  are called the expansion coefficients; the square of their module determines the probability  $P_S(u_i)$  that  $u$  has the value  $u_i$  in the state  $S$ :  $P_S(u_i) = |\sigma_i|^2$ . The square of the module of  $\Psi(\mathbf{q})$  gives the probability that, in the state  $S$ , the system is to be found in position  $\mathbf{q}$ :  $P_S(\mathbf{q}) = |\Psi(\mathbf{q})|^2$ .

The probability of every physical quantity, in the state  $S$ , is determined by the complex function  $\Psi(\mathbf{q})$  together with the first Schrödinger equation, by means of the following two steps:

1. The eigenvalues of the first Schrödinger equation give the admissible values for that physical quantity.
2. The representation of  $\Psi(\mathbf{q})$  as a sum of the eigenfunctions gives, by means of the expansion coefficients, the probability of every value.

**Second Schrödinger equation.**

The second Schrödinger equation describes the time dependence of  $\Psi(\mathbf{q})$ :

$$(3.11) \quad E_{op}\Psi(\mathbf{q},t) = \frac{ih}{2\pi} \frac{\partial\Psi(\mathbf{q},t)}{\partial t}$$

where  $E_{op}$  is the quantum operator for the energy.

If  $\Psi(\mathbf{q})$  is known at a given time, then  $\Psi(\mathbf{q})$  can be calculated at every time in the future and in the past, by means of the second Schrödinger equation. Thus, in the state  $S$ , the probability of every physical quantity is determined in every time.

**A brief recapitulation.**

A quantum state is described by a complex function  $\Psi$ . Every physical quantity is defined by a quantum operator which satisfies the first Schrödinger equation. The eigenvalues determine

the possible value of the quantity. The function  $\Psi$  is represented as a sum of the eigenfunctions; the expansion coefficients give the probability of every possible value of the quantity. The time dependence of  $\Psi$  is described by the second Schrödinger equation, which determines  $\Psi$  at every time. Thus the probability of every admissible value of every physical quantity is determined.

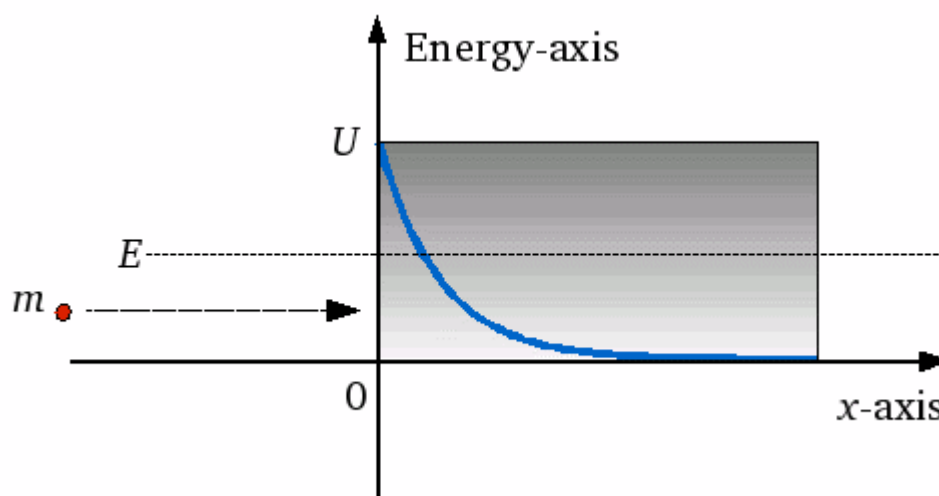
## 4. Applications.

Two applications of Schrödinger equations are presented: the forecast of the tunnel effect and an explanation of [alpha radioactivity](#).

### Tunnel effect.

Consider a particle, with a definite energy  $E$ , moving towards a potential barrier of height  $U > E$ : According to classical mechanics, the particle cannot go through that barrier. On the contrary, in quantum mechanics there is a not null probability that the particle goes through the barrier. This is a consequence of first Schrödinger equation.

In the following, we will study the tunnel effect with respect to a particle moving in only one direction, to simplify the problem from a mathematical point of view.



A particle moving along the  $x$ -axis, with mass  $m$  and energy  $E$ , approaches from the left a potential barrier with energy  $U > E$ . According to classical mechanics, the particle cannot go inside the potential barrier: The grey area in the draw is inaccessible. According to quantum mechanics, the probability that the particle penetrates the potential barrier (blue line in the draw) is not null.

The first Schrödinger equation applied to that particle is:

$$(4.1) \quad \frac{d^2 \varphi(x)}{dx^2} + \frac{2m}{\hbar^2} (E - U) \varphi(x) = 0$$

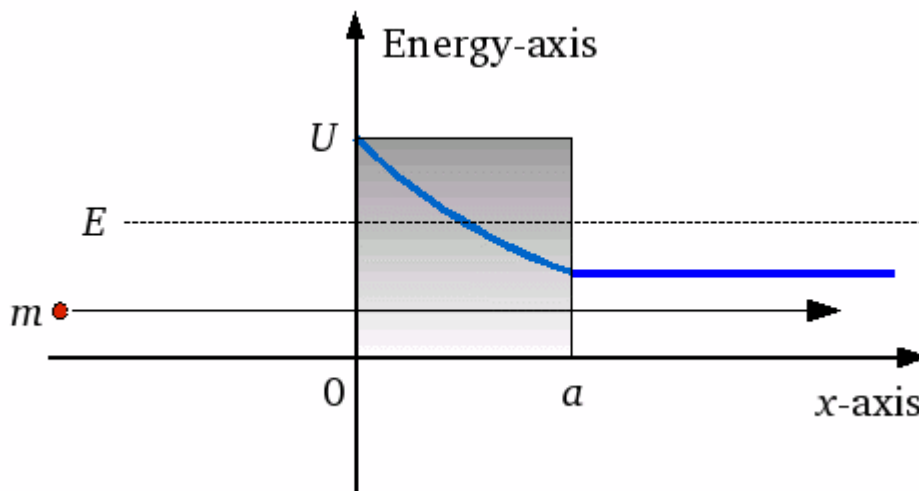
Equation (4.1) is a [linear differential equation](#) with constant coefficients. The auxiliary equation  $k^2 + \frac{2m}{\hbar^2} (E - U) = 0$  has two real solutions:

$$k_1 = +\sqrt{\frac{2m}{\hbar^2} (E - U)} \quad , \quad k_2 = -\sqrt{\frac{2m}{\hbar^2} (E - U)} .$$

Thus two solutions of equation (4.1) are the real functions  $\varphi_1(x) = e^{x k}$  and  $\varphi_2(x) = e^{-x k}$ , where  $e$  is the base of natural logarithms. Since the first divergent solution  $\varphi_1(x)$  is not acceptable, the general solution for equation (4.1) is the real function  $\varphi(x) = A \cdot e^{-x k}$ , where  $A$  is a real arbitrary constant and  $k = \sqrt{\frac{2m}{\hbar^2}(E-U)}$ .

The function  $\varphi(x) = A \cdot e^{-x k}$  describe the state of the particle inside the potential barrier. The square of its module gives the probability  $P(x)$  that the particle is in a point  $x$  occupied by the potential barrier:  $P(x) = |A \cdot e^{-x k}|^2 = A^2 \cdot e^{-2 x k}$ . The probability that the particle is in a point inside the potential barrier is not null. Thus, according to Schrödinger quantum mechanics, a particle can penetrate in a potential barrier in a manner prohibited by classical mechanics.

**Transmission coefficient.**



A particle moving along the  $x$ -axis, with mass  $m$  and energy  $E$ , approaches from the left a potential barrier with energy  $U > E$ . According to quantum mechanics, the probability that the particle penetrates the potential barrier (blue line in the draw) is not null. The transmission coefficient  $T$  is the probability that the particle reaches the point  $a$ , thus passing the potential barrier and penetrating into the region on the right.

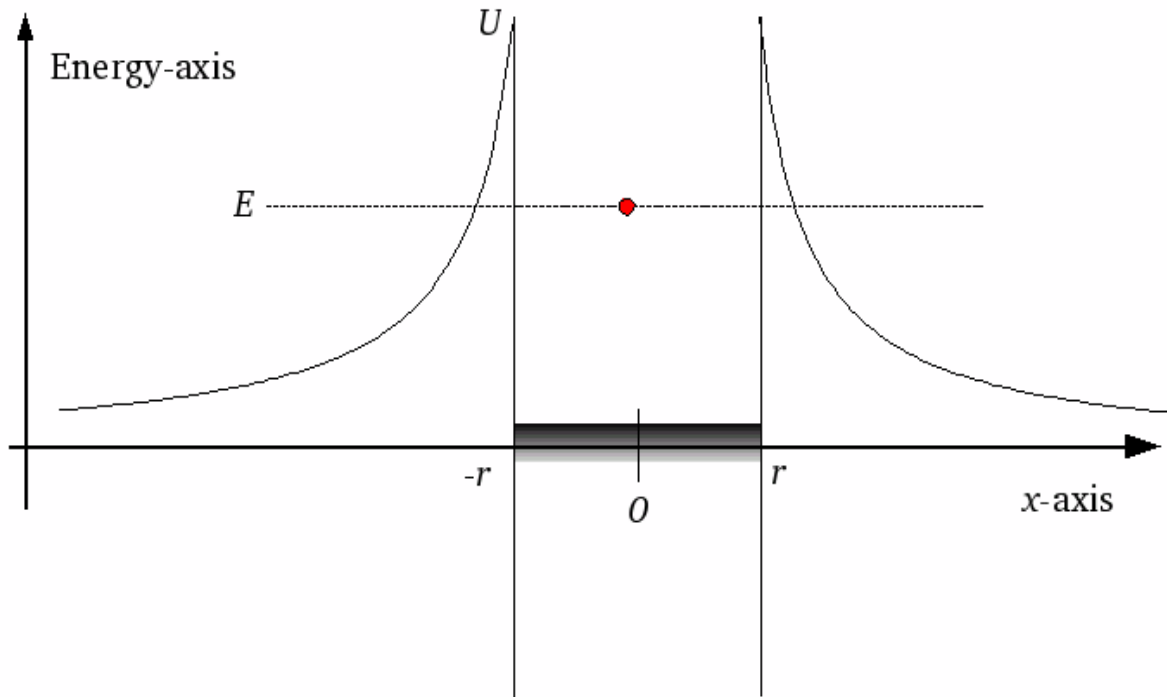
Let  $\varphi(x) = e^{-x k}$  a solution of the first Schrödinger equation applied to the particle inside the potential barrier, where  $k = \sqrt{\frac{2m}{\hbar^2}(E-U)}$ . A rough approximation for the transmission

coefficient is given by the quotient of  $\varphi(a)$  by  $\varphi(0)$ . This quotient is  $e^{-a k}$ ; the square of its module gives the probability that the particle passes the potential barrier. This probability is, by definition, the transmission coefficient. Thus  $T = |\varphi(a) / \varphi(0)|^2 = |e^{-a k}|^2 = e^{-2 a k}$ .

**Alpha radioactivity.**

The alpha decay is a type of radioactive disintegration whereby a parent nucleus, with charge  $Ze$  ( $e$  is the electron charge), breaks up into a decay nucleus, called the daughter, with charge  $(Z-2)e$ , and a helium nucleus, called alpha particle, with charge  $2e$ .

The alpha decay can be explained in terms of the tunnel effect. The figure is a drastically simplified illustration of the situation.



An alpha particle (red dot), with energy  $E$ , is inside a nucleus (gray region of  $x$ -axis), with radius  $r$ . Outside the nucleus (where  $|x| > r$ ) the potential  $U$  is the Coulomb potential:  $U = 2e^2 (Z - 2) / |x|$ . When the alpha particle is outside the nucleus, its measured energy  $E$  is less than the maximum value of  $U = 2e^2 (Z - 2) / |r|$ . Thus the alpha particle is inside a potential well and, according to classical mechanics, its energy is insufficient to escape.

The explanation of alpha radioactivity is possible in terms of the tunnel effect, according to which there is a not null probability that the alpha particle can move through the potential barrier, escaping from the nucleus.

The main difficulty in explaining alpha radioactivity arise from the very large variability of the half life of the emitting substances. From the empirical evidence results that the half life depends on the energy of the emitted alpha particle. This energy varies between 4 MeV and 10 MeV (thus a variation by a factor 2.5) while the half life varies between  $10^{10}$  years ( $=10^{18}$  seconds) and  $0.1 \mu\text{sec}$  ( $=10^{-7}$  seconds), with a variation by a factor  $10^{25}$ . How so a large

variation can be explained, when the energy varies by a small factor?

The transmission coefficient, that is the probability that the alpha particle escapes from the nucleus, is correlated with the half life of the emitting nucleus. The theory of the tunnel effect enables us to calculate the transmission coefficient; using some drastic simplifications, the following relation, which connects the half life  $\tau$  and the energy  $E$  of the alpha particle, can be obtained:

$$(4.2) \quad \text{Log}(\tau) = (148 / \sqrt{E}) - 53.5$$

where  $\tau$  is measured in seconds and  $E$  in MeV. Calculating the equation (4.2) for the values  $E = 4$  MeV and  $E = 10$  MeV we obtain:

$$\text{for } E = 4 \text{ MeV} : \text{Log}(\tau) = (148 / \sqrt{4}) - 53.5 = 20.5$$

$$\text{for } E = 10 \text{ MeV} : \text{Log}(\tau) = (148 / \sqrt{10}) - 53.5 = -6.7$$

The logarithm of the half life shows a variation of about 27; thus the half life shows a variation by a factor  $10^{27}$ . Hence a small variation in the energy of the alpha particle can explain the very large amount of variability of the half life of the emitting substances.

## 5. Heisenberg indeterminacy principle.

The section begins with the distinction between commutative and non commutative operators. The role of this distinction, which is a main feature of quantum mechanics, is illustrated by the analysis of measurement in quantum mechanics. A brief explanation of Ehrenfest theorem on mean values precedes the formulation of Heisenberg indeterminacy principle. The section ends with some physical applications of Heisenberg indeterminacy principle.

### Commutative operators.

Let  $u$  and  $v$  be two physical quantities, and let  $u_{op}$  and  $v_{op}$  be the associated quantum operators. Suppose that  $u_{op}$  is applied to a complex function  $\varphi$  to construct the function  $u_{op} \varphi$ . It is possible to apply  $v_{op}$  to that function and obtain  $v_{op} u_{op} \varphi$ ; this expression indicates the application of operator  $u_{op}$  to the function  $\varphi$ , followed by the application of operator  $v_{op}$  to the resulting function.

The question arise whether the order of application of quantum operators is essential:  $v_{op} u_{op} \varphi$  is the same as  $u_{op} v_{op} \varphi$ ? If you remember the meaning of  $u_{op} v_{op} \varphi$ , which is not a multiplication of number, but an application of quantum operators to transform a function in another function, you can guess that in general  $v_{op} u_{op} \varphi$  is not the same as  $u_{op} v_{op} \varphi$ . However, for some quantum operators  $u_{op}$  and  $v_{op}$ , the following relation holds:

$$(5.1) \quad v_{op} u_{op} \varphi = u_{op} v_{op} \varphi$$

Two particular quantum operators for which the relation (5.1) is true for every function  $\varphi$  are called commutative operators, and the corresponding physical quantities are called commutative entities. Note that the notion of commutative operators is applicable only to a pair of quantum operators: An operator is commutative with respect to another operators.

An as example of a pair of commutative quantum operators, consider the position  $q_1$  and the momentum  $p_2$ ; note that they are referred to two different axes. We have:

$$\begin{aligned} q_{1op} p_{2op} \varphi - p_{2op} q_{1op} \varphi &= q_{1op} \frac{\hbar}{2\pi i} \frac{\partial \varphi}{\partial q_2} - p_{2op} q_1 \varphi = \\ &= q_1 \frac{\hbar}{2\pi i} \frac{\partial \varphi}{\partial q_2} - \frac{\hbar}{2\pi i} \frac{\partial q_1 \varphi}{\partial q_2} = q_1 \frac{\hbar}{2\pi i} \frac{\partial \varphi}{\partial q_2} - q_1 \frac{\hbar}{2\pi i} \frac{\partial \varphi}{\partial q_2} = 0 \end{aligned}$$

There is an important property which holds for a pair of commutative entities: Two commutative entities have the same set of eigenfunctions.

### Non commutative operators.

Two quantum operators  $u_{op}$  and  $v_{op}$  are called non commutative if exists a function  $\varphi$  such that  $u_{op} v_{op} \varphi \neq v_{op} u_{op} \varphi$ . A typical example of non commutative quantum operators is given by position and momentum operators, when they are referred to the same axis. We have:

$$\begin{aligned}
 q_{1\text{op}} p_{1\text{op}} \varphi - p_{1\text{op}} q_{1\text{op}} \varphi &= q_{1\text{op}} \frac{\hbar}{2\pi i} \frac{\partial \varphi}{\partial q_1} - p_{1\text{op}} q_1 \varphi = \\
 &= q_1 \frac{\hbar}{2\pi i} \frac{\partial \varphi}{\partial q_1} - \frac{\hbar}{2\pi i} \frac{\partial q_1 \varphi}{\partial q_1} = q_1 \frac{\hbar}{2\pi i} \frac{\partial \varphi}{\partial q_1} - \frac{\hbar}{2\pi i} (q_1 \frac{\partial \varphi}{\partial q_1} + \varphi) = \\
 &= q_1 \frac{\hbar}{2\pi i} \frac{\partial \varphi}{\partial q_1} - q_1 \frac{\hbar}{2\pi i} \frac{\partial \varphi}{\partial q_1} - \frac{\hbar}{2\pi i} \varphi = -\frac{\hbar}{2\pi i} \varphi
 \end{aligned}$$

Assuming that  $p$  and  $q$  are referred to the same axis, this relation can be written as

$$(q_{\text{op}} p_{\text{op}} - p_{\text{op}} q_{\text{op}}) \varphi = \frac{\hbar}{2\pi i} \varphi = \frac{\hbar}{i} \varphi = -\hbar i \varphi$$

Note that the notion of non commutative operators is applicable only to a pair of quantum operators: An operator is non commutative with respect to another operators.

Two non commutative entities have different set of eigenfunctions.

### The effect of measurement on $\Psi$ function.

The state of a quantum system is described by a function  $\Psi(\mathbf{q})$  that can be represented as a sum of the eigenfunctions of a physical quantity  $u$ :

$$(5.2) \quad \Psi(\mathbf{q}) = \sum_{i=1}^{i=\infty} \sigma_i \cdot \varphi_i(\mathbf{q})$$

where the square of the module of the expansion coefficients  $\sigma_i$  determines the probability that  $u$  has the value  $u_i$ .

Let  $u$  and  $v$  two non commutative physical quantities; they have two different sets of eigenfunctions. Suppose that a measurement of  $u$  is performed, and the resulting value for  $u$  is  $u_k$ . Thus the probability that  $u$  has the value  $u_k$  is equal to 1. Hence  $\sigma_k = 1$  and  $\sigma_i = 0$  for every  $i \neq k$ . The equation (5.2) becomes  $\Psi^u(\mathbf{q}) = \varphi_k^u(\mathbf{q})$  (the superscript  $u$  in the equation marks the fact that the state of the system is determined immediately after a measurement of  $u$ ).

Immediately after the measurement of  $u$ , a measurement of  $v$  is performed; the result is  $v_h$  and thus equation (5.2) becomes  $\Psi^v(\mathbf{q}) = \varphi_h^v(\mathbf{q})$ . Since  $u$  and  $v$  have different sets of eigenfunctions, we have  $\varphi_k^u(\mathbf{q}) \neq \varphi_h^v(\mathbf{q})$  and thus  $\Psi^u(\mathbf{q}) \neq \Psi^v(\mathbf{q})$ . A measurement of  $v$ , performed after the measurement of a non commutative quantity  $u$ , changes the function describing the state of the system.



The measurement of a quantity determines a function  $\Psi$  describing the quantum system. If, immediately after this measurement, another one is performed on a non commutative quantity, a different function  $\Psi$  is determined. Since function  $\Psi$  completely describes the status of the system, we must conclude that the second measurement has altered the state of the system. The situation is different if we consider two commutative entities, since they have the same set of eigenfunctions.

We can summarize the situation in the following way: In a quantum system, described by a function  $\Psi$  defined as the sum of the eigenfunctions of an entity, the measurement of a commutative entity does not alter the state of the system, while the measurement of a non commutative entity does alter the state of the system.

A consequence of the fact that two non commutative entities have different sets of eigenfunctions is that there is no functions  $\Psi$  which, as the same time, can be written as the sum of the eigenfunctions of two non commutative entities. Thus there is no physical state corresponding to a quantum system in which two commutative entities have, at the same time, definite unique values. If  $u$  and  $v$  are non commutative entities, then there is no quantum system in which  $u(t) = u_o$  and  $v(t) = v_o$  for the same time  $t$ . As an example, consider a quantum particle moving along the  $x$ -axis; there is no physical state of this particle corresponding to the situation in which the particle has a definite position and definite momentum in the same time. As an obvious consequence, it is impossible to measure the exact position and momentum of a quantum particle, since there is no physical state corresponding to such measurement: There is nothing such as an exact position and momentum of a quantum particle. The impossibility of a such kind of measurement is not a human limitation, but it is a limitation of the applicability of classical concepts, which assign a definite position and momentum to a particle. In quantum mechanics the concept of the path of a particle is not applicable; it is only a classical notion, used as a first approximation, that in some circumstances is inadequate.

### Mean values.

The mean value (also known as the expectation or the expected value)  $E(u)$  of a physical quantity  $u$  can be calculated from the function  $\Psi$  using the following formula, where  $u_{op}$  is the quantum operator associated to  $u$ :

$$(5.3) \quad E(u) = \int_{-\infty}^{+\infty} \Psi^*(x) u_{op} \Psi(x) dx$$

In equation (5.3) the operator  $u_{op}$  acts on function  $\Psi$ . We can also calculate the mean value of  $u^2$  using the formula

$$(5.4) \quad E(u^2) = \int_{-\infty}^{+\infty} \Psi^*(x) u_{op}^2 \Psi(x) dx$$

The indetermination  $\Delta u$  of  $u$  is given by the equation  $(\Delta u)^2 = \mathbf{E}(u^2) - [\mathbf{E}(u)]^2$ . A theorem, due to Paul Ehrenfest, states that the mean values of position and momentum of a particle with mass  $m$  satisfy the equations of classical mechanics:

$$(5.5) \quad \frac{d}{dt}\mathbf{E}(q_i) = \frac{1}{m}\mathbf{E}(p_i) , \quad \frac{d}{dt}\mathbf{E}(p_i) = -\mathbf{E}\left(\frac{dV(q_i)}{dq_i}\right)$$

Equation (5.5) gives a connection between quantum mechanics and classical mechanics. If the indetermination of position and momentum of a particle is so small that it can be ignored, then the particle acts according to the classical laws of motion.

The amount of the indetermination is given by Heisenberg indeterminacy principle, which affirms that the indetermination  $\Delta u$  and  $\Delta v$  of two non commutative entities satisfy the relation

$$(5.6) \quad \Delta u \Delta v \geq \hbar$$

If the non commutative entities are position and momentum, the equation (5.6) becomes

$$(5.7) \quad \Delta q_i \Delta p_i \geq \hbar \approx 1 \text{ erg}^{-27} \text{ sec}$$

*Note: 1 erg is the energy of a particle having a mass of 1 gm and a velocity of 1 cm/sec.*

Equations (5.7) and (5.5) explain the success of classical mechanics in the realm of macroscopic objects.

### **Applications of the indeterminacy principle.**

We can use Heisenberg indeterminacy principle to understand why a quantum particle is able to escape from a potential well. The position  $q$  of the particle inside a potential well is strongly localized, thus the indetermination of its momentum  $p$  is high. Since the kinetic energy  $T$  of the particle is a function of its momentum  $p$  ( $T = p^2/2m$ ), the indetermination of the energy is high too. As a consequence of this indetermination, the particle can have enough energy to escape.

Another application of the indeterminacy principle concerns the zero-point energy. A quantum particle cannot be completely at rest, because in such case the indetermination of its position and momentum will be zero. This is true also for a particle at absolute zero. In classical physics, a particle at absolute zero has no energy at all; in quantum mechanics, a particle at absolute zero is not at rest, so it has a residual energy.

The indeterminacy principle is applicable also to energy  $E$  and time  $t$ :

$$(5.8) \quad \Delta E \Delta t \geq \hbar$$

## HEISENBERG INDETERMINACY PRINCIPLE

When applied to the electromagnetic field, formula (5.8) states that also in empty space the electromagnetic field has an energy, called the vacuum energy. Given the equivalence between energy and mass, the vacuum energy can manifest itself creating couples of short-lived particles and anti-particles, which disappear in a time interval  $t$  determined by equation (5.8).



## 6. Links and further reading.

### Physics.

- Suranyi, Peter. "Lecture Notes in Modern Physics" *University of Cincinnati, Department of Physics* [URL:http://physuna.phs.uc.edu/suranyi/Modern\\_physics/Lecture\\_Notes/lecture\\_notes.html](http://physuna.phs.uc.edu/suranyi/Modern_physics/Lecture_Notes/lecture_notes.html) [Accessed January 24, 2005]
- Takada, Kenjiro. "Internet Seminar Microscopic World -2- (Introduction to Quantum Mechanics)" *Experimental Nuclear Physics, Kyushu University* [URL:http://www2.kutl.kyushu-u.ac.jp/seminar/MicroWorld2\\_E/MicroWorld\\_2\\_E.html](http://www2.kutl.kyushu-u.ac.jp/seminar/MicroWorld2_E/MicroWorld_2_E.html) [Accessed January 24, 2005]

### Philosophy.

- Hájek, Alan. "Interpretations of Probability" *The Stanford Encyclopedia of Philosophy (Summer 2003 Edition)* Edward N. Zalta (ed.) [URL:http://plato.stanford.edu/archives/sum2003/entries/probability-interpret/](http://plato.stanford.edu/archives/sum2003/entries/probability-interpret/) [Accessed January 24, 2005]
- Hilgevoord, Jan, Uffink, Jos. "The Uncertainty Principle" *The Stanford Encyclopedia of Philosophy (Winter 2001 Edition)* Edward N. Zalta (ed.) [URL:http://plato.stanford.edu/archives/win2001/entries/qt-uncertainty/](http://plato.stanford.edu/archives/win2001/entries/qt-uncertainty/) [Accessed January 30, 2005]
- Ismael, Jenann. "Quantum Mechanics" *The Stanford Encyclopedia of Philosophy (Fall 2004 Edition)* Edward N. Zalta (ed.) [URL:http://plato.stanford.edu/archives/fall2004/entries/qm/](http://plato.stanford.edu/archives/fall2004/entries/qm/) [Accessed January 24, 2005]
- Krips, Henry. "Measurement in Quantum Theory" *The Stanford Encyclopedia of Philosophy (Winter 1999 Edition)* Edward N. Zalta (ed.) [URL:http://plato.stanford.edu/archives/win1999/entries/qt-measurement/](http://plato.stanford.edu/archives/win1999/entries/qt-measurement/) [Accessed January 24, 2005]
- Murzi, Mauro. "Reichenbach, Hans" *Internet Encyclopedia of Philosophy* [URL:http://www.iep.utm.edu/r/reichenb.htm](http://www.iep.utm.edu/r/reichenb.htm) [Accessed December 30, 2004]
- Wilce, Alexander. "Quantum Logic and Probability Theory" *The Stanford Encyclopedia of Philosophy (Spring 2003 Edition)* Edward N. Zalta (ed.) [URL:http://plato.stanford.edu/archives/spr2003/entries/qt-quantlog/](http://plato.stanford.edu/archives/spr2003/entries/qt-quantlog/) [Accessed January 24, 2005]

### Further reading.

- Gamow, George. *Thirty Years That Shook Physics: The Story of Quantum Theory*. Dover, 1985 (originally published in 1966).
- Hund, Friedrich. *The history of quantum theory*. Harrap, 1974.
- Jammer, Max. *The Philosophy of Quantum Mechanics*. John Wiley & Sons, 1974.
- Reichenbach, Hans. *Philosophic Foundations of Quantum Mechanics*. Dover, 1998 (originally published in 1944).
- Wichmann, Eyvind H. *Quantum physics (Berkeley physics course)*. McGraw-Hill, 1967, 1971



## Appendix

### Linear differential equations.

A second order linear differential equation with constant coefficients is an equation of the type:

$$(D.1) \quad a \frac{d^2 f(x)}{dx^2} + b \frac{df(x)}{dx} + c f(x) = 0$$

where  $a$ ,  $b$  and  $c$  are real numbers.

Finding functions  $f(x)$  solutions of this kind of equations is simple. Consider the second order equation  $a \cdot k^2 + b \cdot k + c = 0$ , called the characteristic equation, and let  $k_1$  and  $k_2$  be its solution.

There are three different cases:

1.  $k_1$  and  $k_2$  are different real numbers. Two particular solutions of equation (D.1) are  $f_1(x) = e^{x k_1}$  and  $f_2(x) = e^{x k_2}$ .
2.  $k_1$  and  $k_2$  are equal real numbers. Two particular solutions of equation (D.1) are  $f_1(x) = e^{x k_1}$  and  $f_2(x) = x \cdot e^{x k_1}$ .
3.  $k_1$  and  $k_2$  are different complex numbers:  $k_1 = p + iq$ ,  $k_2 = p - iq$ . Two particular solutions of equation (D.1) are  $f_1(x) = e^{p x} \cos(qx)$  and  $f_2(x) = e^{p x} \sin(qx)$ .

The general solution of equation (D.1) is a linear combination of two particular solutions:  $f(x) = A \cdot f_1(x) + B \cdot f_2(x)$ , where  $A$  and  $B$  are real numbers.