"Enrico Fermi" Chair
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A History of the Science of Light

From Galileo's telescope to the laser and the quantum information technologies

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Lecture 5. February 24th 2022

Lecture 5:
The theoretical framework of quantum theory and its physical interpretation

Outline of lecture:

1. The introduction of matter waves by de Broglie, inspired by Einstein's special relativity and photon theory. Recovering Boh's quantization rules of Hydrogen atom with de Broglie waves.

2. Discovery of Schrödinger's equation describing the evolution of the matter waves. Extension of this equation to a many-particle system. The probabilistic interpretation of the wave function. Remark about the non-relativistic nature of this equation (see the relativistic Dirac equation in Lecture 7).

3. Heisenberg uncertainty relations and Bohr's complementarity principle. Tests of uncertainty relations and complementarity by thought experiments. Consequences of Heisenberg uncertainty relations for stability of atoms and relationship between the phase and the amplitude of an oscillator

4. Description of the modern quantum theory using the bra-ket Dirac formalism: Hilbert space of quantum states, superposition principle. Physical obervables represented by operators acting in the Hilbert space. Eigenstates and eigenvalues of obervables and their spectrum. The measurement postulates of quantum physics. The wave function as a special representation of quantum states of particles moving in space. Translation in space, momentum and time of quantum states.

The veil is lifted on quanta: Matter waves

A few weeks after learning about Bose's work, Einstein received in 1924 a letter from Langevin informing him about the work of his student, Louis de Broglie who had suggested that all particles, not only photons, have a wave like-character. Einstein recognized the importance of this work and the connection which could be made with the phenomenon of Bose—Einstein condensation that he had just discovered. He wrote to Langevin:

« de Broglie's thesis has lifted a corner of the great veil »

and to Lorentz:

« The young de Broglie has made a very interesting attempt to interpret the Bohr-Sommerfeld quantization rules. I think it is the first ray of weak light to illuminate these rules, the worst of our physical puzzles. I have also discovered something which supports this construction »

Einstein and Langevin in 1922 at the Collège de France

De Broglie intuition had come from both Einstein's 1905 photon and relativity papers which he had studied in details. It is thus natural that this new revolutionary idea resonated immediately with Einstein.

De Broglie in 1929

De Broglie wavelength of a massive particle

De Broglie extrapolated the relation between the photon momentum and wavelength to matter particles:

Massless photon of momentum p=hν/c

$$\lambda = \frac{c}{\nu} = \frac{h}{(h\nu/c)} = \frac{h}{p}$$

Matter particle of mass m and velocity v (electron, atom etc)

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

This « heuristic analogy » compares the property of an intrinsicaly relativistic particle (the photon) with that of non-relativistic massive particles. A free particle moving with momentum **p**=m**V** is associated to a plane wave whose spatial dependence at a given time writes in complex notation:

$\psi \sim e^{2i\pi x/\lambda} = e^{ipx/\hbar}$ if the particle moves along Ox; $\psi \sim e^{i\vec{p}.\vec{r}/\hbar}$ if its momentum is oriented along an arbitrary direction

One recognize in the phase of this wave the momentum-space contribution of the 4-D scalar product introduced in relativity theory. This suggests immediately to add the time dependence of the wave and to write it as:

$$\psi(\vec{r},t) \sim e^{-i(Et-\vec{p}.\vec{r})/\hbar}$$

where E, the energy of the free particle, is equal to $p^2/2m$ at the non-relativistic limit (v<<c).

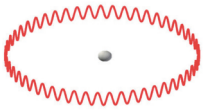
Matter waves explain Bohr's quantization rule

Bohr's quantization rule of the electron angular momentum in hydrogen writes:

$$mvr = n\hbar$$

which can be expressed as:

$$2\pi r = n\lambda_{dB} \quad with \quad \lambda_{dB} = h/mv$$



The n^{th} Bohr orbit described as a de Broglie wave rotating on a circle and interfering constructively with itself after a revolution (here n=50)

The quantization expresses the tact that there must be an integer number of electronic de Broglie wavelengths on the orbit circumference: this appears as a resonance condition analogous to the ones encountered with vibrating springs or electromagentic radiation between mirrors. The principal number of Bohr's theory is merely the number of de Broglie wavelenths accomodated along the orbit circumference. The Schrödinger equation will show that in fact, the electron angular momentum on the circular orbit is equal to n-1, not to n.

De Broglie wavelength and the threshold of BEC

Einstein understood that de Broglie matter wave hypothesis gave a clear physical interpretation of the BEC condensation phenomenon. For his calculation of the saturation of the ideal gas , he had assumed that the phase space (**r**,**p**) of the atoms was divided into elementary cells of volume h^3. This calculation yielded a critical atomic density (see lecture 4):

$$N/V = \xi\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} \qquad with\ \xi = 2.61..$$

He realized that the quantity in the bracket was the inverse of the cube of a de Broglie wavelength:

$$\lambda_{th} = \left(\frac{h^2}{2\pi m k_B T}\right)^{\frac{1}{2}}$$

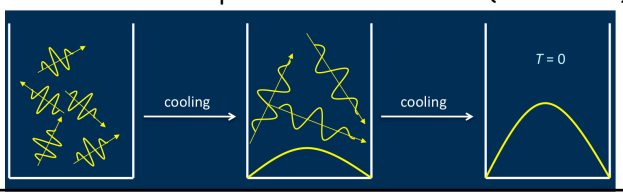
which corresponds to atoms moving in the gas with an average velocity:

$$v_{th} = h/m\lambda_{th} = \sqrt{2\pi k_B T/m}$$

of the order of the rms velocity in an ideal gas at temperature T (v_{rms}= $(3k_BT/m)^{1/2}$).

BEC starts when the atomic density of the saturated phase (called also the thermal phase) becomes of the order of 1 atom per λ^3. The waves of neighbouring atoms start to overlap and more and more atoms fall in the ground state.

When T decreases, the atomic de Broglie wavelength increases to the point of condensation (few 100 nK)



If there is a wave, what is its equation?

(Debye's question after a seminar in which Schrödinger presented de Broglie's work in Zurich)

To find the propagation equation for a free particle, take the sum of the second derivatives with respect to space and compare to the first derivative with respect to time.

$$\Delta\psi = -\frac{p^2}{\hbar^2}\psi \quad with \quad \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (Laplacian)$$

$$i\hbar\frac{\partial\psi}{\partial t} = E\psi = \frac{p^2}{2m}\psi$$

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi}$$

Schrödinger equation for a free particle

To find the propagation equation of a particle in a time independent potential, just add the energy potential to the Laplacian term representing the kinetic energy

$$E = \frac{p^2}{2m} + U(\vec{r}) \rightarrow i\hbar\frac{\partial}{\partial t} = -\frac{\hbar^2}{2m}\Delta + U(\vec{r})$$

$$\boxed{i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = U(\vec{r})\psi(\vec{r},t) - \frac{\hbar^2}{2m}\Delta\psi(\vec{r},t)}$$

Schrödinger equation for a particle in a potential

The Schrödinger equation

The derivation outlined above is not a demonstration. A more elaborate justification of Schrödinger's equation (SE) can be given based on the Hamilton-Jacobi version of classical mechanics, by considering that quantum mechanics is related to classical physics in the same way as wave optics is an extension of ray optics. This is the route that Schrödinger followed to establish his equation. Its true justification is its success: when extended to multiparticle systems, its solutions – exact or numerical - fit with experimental observations in physics (structure of atoms, condensed matter) and in chemistry (structure of molecules, chemical reactions). In fact, SE must be accepted, with its probabilistic interpretation, as a postulate of non-relativistic quantum physics.

Extended to n interacting particles of masses m_i at positions $\mathbf{r}_i$, ψ becomes a function of n+1 variables (n positions + time) which obeys the generalized Schrödinger equation:

$$ih\frac{\partial\psi(\vec{r}_1,\vec{r}_2,\cdots\vec{r}_n,t)}{\partial t} = \left[-\sum_i \frac{\hbar^2}{2m_i}\Delta_i + U(\vec{r}_1,\vec{r}_2,\cdots\vec{r}_n)\right]\psi(\vec{r}_1,\vec{r}_2,\cdots\vec{r}_n,t)$$

The differential operator in the bracket is the system's Hamiltonian

This equation is linear in ψ which means that if ψ_1 and ψ_2 are solutions, then $a_1\psi_1+a_2\psi_2$ is also a solution for arbitrary complex a_1 and a_2. This expresses the **superposition principle** of quantum physics: the matter waves can combine and interfere as light waves do in Maxwell's theory.

Although based on extrapolation of photon properties, SE is not relativistic. Time and space do not play symmetrical roles (1st derivative for time, 2nd for space). A relativistic equation for the electron was derived one year later by Dirac, predicting t the electron spin and the positron. (see Lecture 6).

The probabilistic interpretation of the wave function (Born-1925)

$$\left|\psi(\vec{r}_1 \cdots \vec{r}_n)\right|^2 d^3r_1 \cdots d^3r_1$$

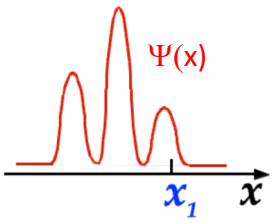
Joint probability to find the particles in small volume elements $d^3r_1 \cdots d^3r$ around positions $\vec{r}_1 \cdots \vec{r}_n$

$$\int \left|\psi(\vec{r}_1 \cdots \vec{r}_n)\right|^2 d^3r_1 \cdots d^3r_n = 1$$

Chance becomes an essential feature of quantum physics. Theory predicts only probabilities to find results when measurements are performed.

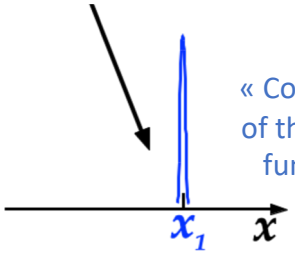
The evolution equation is deterministic as long as no attempt is made to perform a measurement, but system undergoes a random change when a measurement is made.

Measurement changes the wave function in a random way



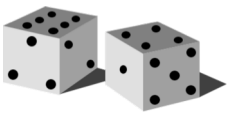
Particle measured at position x_1

Probability $P(x_1) = |\Psi(x_1)|^2$



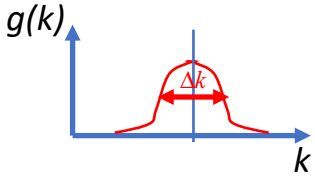
« Collapse » of the wave function

In quantum physics « God is paying dice »



Einstein did not like this….

Fourier transform of a wave packet



Consider a wave packet of plane em waves propagating along Oz :

$$f(z,t) = \int g(k) e^{i(kz-\omega t)}\, dk$$

The angular frequency ω and wave vector k obey the dispersion relation: $\omega = ck$

The spectral width of the wave packet is: $\Delta\omega = c\Delta k$

Assume that all the waves of the packet are in phase at z=t=0. Let us describe the spatial dependence of the packet at t=0. As z departs from z=0, the exp(ikz) components of the wave packet corresponding to different k's accumulate different phases. The interference reduces notably the wave intensity when z departs from 0 by an amount Δz such that:

$$\Delta k \Delta z \sim 1$$

Consider now the time evolution of the wave at z=0. The exp(-iωt) components get also dephased as t departs from zero and the wave decreases notably for:

$$\Delta\omega \Delta t \sim 1$$

The expansion of the wave packet *f* (z,t) into monochromatic waves exp(i(kz-ωt) is a Fourier integral. The f and g functions are Fourier transform of each other. The condition of positive interference is satisfied at all space time points such kz-ωt=0. The wave packet is thus propagating at the speed of light, without changing shape. Its spatial extension is of the order of $1/\Delta k$ and its time duration at each point is of the order of $1/\Delta\omega$. *The extension in space and time of the wave packet are inversely proportional to the widths of the wave vector and angular frequancy distributions. This is a fundamental property of Fourier transforms.*

Heisenberg uncertainty relations

A wave packet associated to a free particle is a sum of plane waves with a distribution of momenta around a central value p_0. The situation is comparable to a light wave packet, sum of monochromatic waves with wave vectors distributed around a central value k_0. Matter and light packets differ by their dispersion relation (linear in optics, quadratic in non relativistic wave mechanics):

Wave mechanics $$\psi(\vec{r},t) = \int g(\vec{p}) e^{i(E_p t - p.r)/\hbar} d^3p\,; \quad E_p = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \quad with\ k = \frac{p}{\hbar} = \frac{2\pi}{\lambda_{dB}}$$

Wave optics $$A_c(\vec{r},t) = \int g(\vec{k}) e^{i(\omega_k t - \vec{k}.\vec{r})} d^3k \quad ; \quad \omega_k = c|k|$$

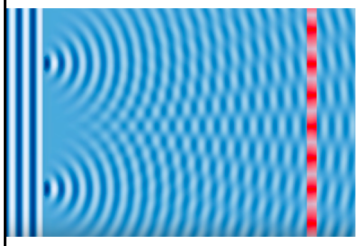
At a given time, ψ and A are respectively the Fourier transforms of g(p) and g(k). The spatial extension of these functions are inversely proportional to that of their Fourier transforms (k or p distributions). If the waves propagate along the x direction, this implies that the product of the wave-vectors and position dispersion along x is of the order of unity.

$\Delta x \Delta k \sim 1$ in optics becomes $\Delta x \Delta p \sim \hbar$ in quantum physics with similar relations along Oy & Oz

A classical mathematics property takes a deep quantum meaning: the better is a particle localized in space, the less well known is its momentum, hence its velocity. The better its velocity is defined, the more diffuse is its position

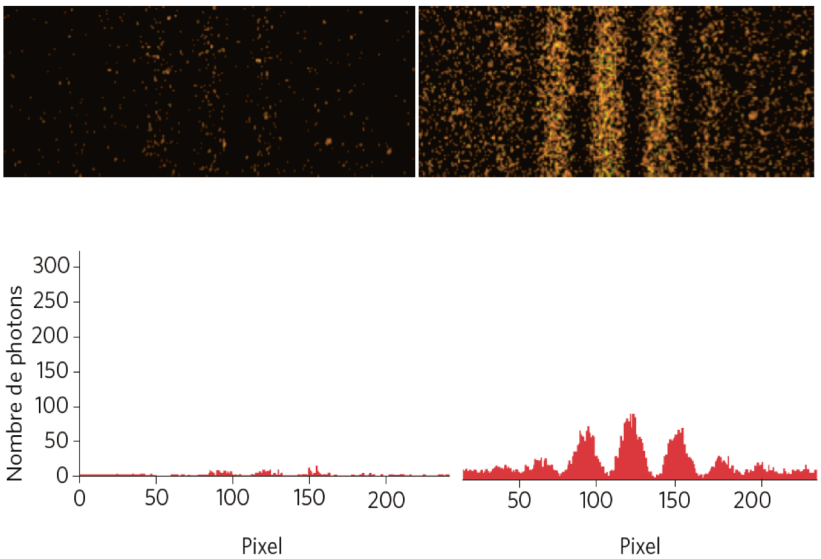
Revisiting the Young double slit experiment: Uncertainty relations and complementarity

Young double-slit experiment can be realized with photons but also with particles (electrons, atoms, molecules etc..)

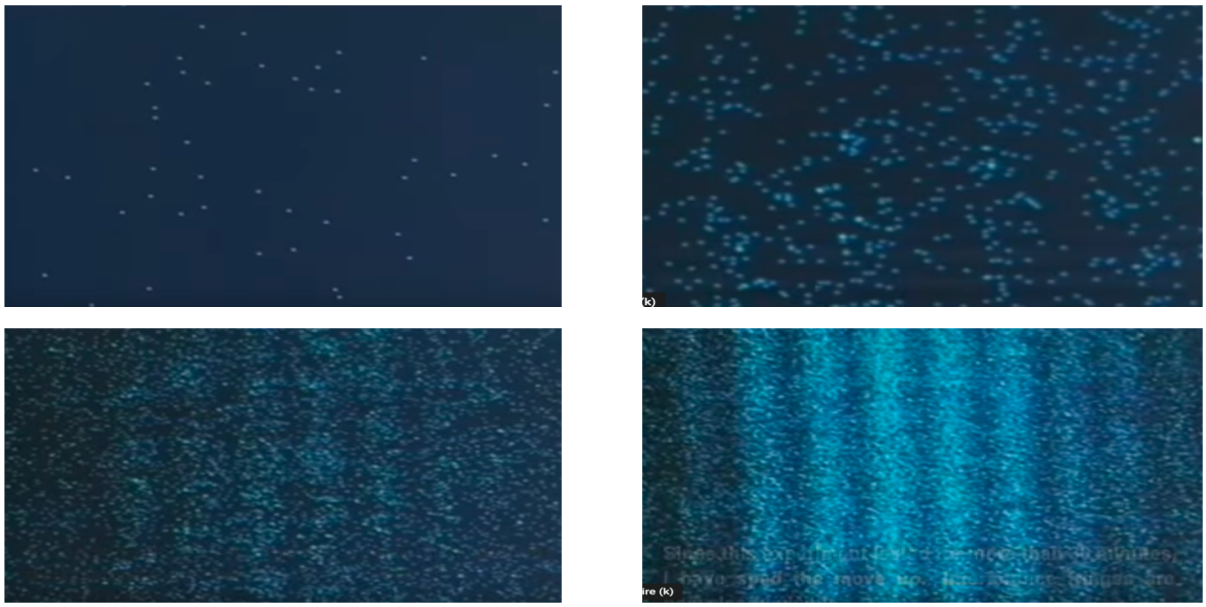


The statistical interpretation is simple: a plane wave (made of photons or massive particles) is diffracted by the slits, forming two secondary waves which interfere constructively along the directions where they are in phase (path difference equal to multiple of wavelengths), destructively along directions where they are in phase opposition (path difference equal to odd multiples of half wave-lengths). The particles impinge randomly on the detection screen at points where the probability amplitudes interfere constructively (bright fringes) and never fall where the interference is destructive (dark fringes).

This experiment can now be performed with sources sending particles one at a time. The interferences are then building up progressively as more and more particles are detected on the screen (see next two slides), In the 1920's these were thought experiments whose interpretation puzzled the founders of the quantum theory and gave rise to heated debates about the wave-particle duality, notably between Bohr and Einstein. These discussions helped Bohr to develop his principle of complementarity in relation with the Heisenberg uncertainty principle.



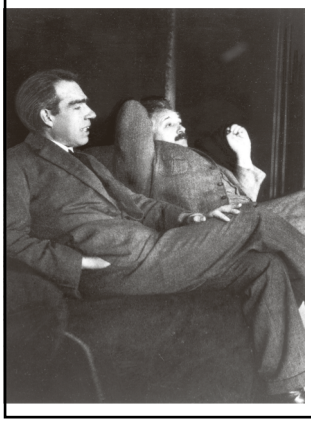
Fresnel biprism interference experiment (equivalent to Young double slit) with a single photon source (J-F Roch)



Electron interferences: progressive build-up of fringes when particles cross apparatus (biprism) one at a time (Tonomura)

Puzzling questions about a simple experiment

The fringe pattern is an interference phenomenon illustrating the superposition principle of quantum theory. The fringes are observed only if both slits are open. When the experiment is performed with one particle at a time, it raises puzzling questions for physicists used to think in terms of Newtonian trajectories:



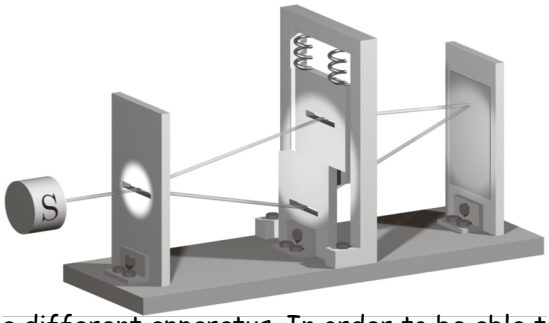
If each particle passes through one hole or the other, how can its subsequent history depend on whether the other slit was open or closed?

How can the particle « know » what is the state of the other slit to « decide » whether or not it can arrive on a dark fringe?

What happens if we decide, without blocking one of the slits, to observe through which one did the particle pass?

The moving slit thought experiment

Einstein: Let us put the upper slit on a moving screen suspended to a spring. If the particle passes through, it will be diffracted and the recoil will set the spring in motion. We will then now through which slit the particle went, without blocking it. Will we then see the fringes?



Bohr: This is a different experiment, with a different apparatus. In order to be able to detect the small change in momentum experienced by the slit, its initial momentum must be very well defined, with an uncertainty Δp smaller than the change which will be produced by the crossing particle. The position of the slit will then be blurred by an amount at least equal to $\Delta x = \hbar / \Delta p$ This uncertainty will modify the difference between the two pathes and wash out the fringe pattern. Thus, the Heisenberg uncertainty principle makes it impossible to know the trajectory of the particle and to oberve its wave nature at the same time (more about this later).

If fringes are observed, the trajectory has no physical reality: the particle crossed the screen in a superposition state, going through the two slits at the same time (more precisely, its wave function did it).

Bohr's complementarity

Speaking about the trajectory of a particle has no meaning, unless the experiment is designed to observe it. If the apparatus can perform the measurement of the position of the particle, it perturbs it in such a way that the wave aspect vanishes and all information about the phase of the matter wave is lost. If on the other hand the fringes are observable, the experimental apparatus cannot provide information about the trajectory. Observing trajectories or interfering patterns are two complementary aspects of the physical reality which require different experimental procedures and equipment.The measurement always perturbs the system by the amount necessary to ensure that the complementarity principle is satisfied.

The trajectory of a particle in an interferopmeter has no reality unless the experiment is modified to provide the required information. If this modification is made, it is not even necessary that this information be registered. The mere fact that the information could be obtained means that the apparatus perturbs enough the system to make the interferences disappear.

This principle extends to other kinds of measurements performed to measure complementary observables about which it is impossible to obtain simultaneous information (see below spin systems).

Bohr's complementarity is not an independent postulate of quantum physics. It expresses in words what is implied by the mathematical rules, established at the end of the 1920's by Heisenberg, Schrödinger, Born, Dirac and von Neumann (see below). Complementary experiments are designed to focus on conjugate observables described by operators which do not commute and cannot be measured simultaneously in a given experiment.

Heisenberg time-energy uncertainty relation

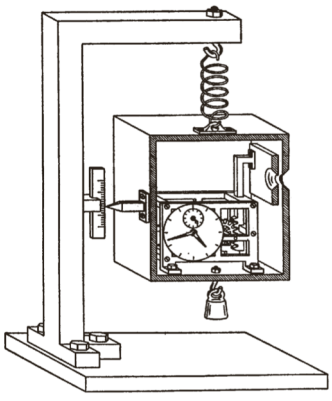
The properties of Fourier transform relate the width of the time and energy distributions of a particle's wave function by the same uncertainty relation as its position and momentum:

$$\Delta E \Delta t \sim \hbar$$

This relation is analogous to the one we have established for a light wave packet (slide above): $\Delta\omega\Delta t = 1$. It means that if a photon is created within a time interval whose duration has the uncertainty Δt, its energy will be defined within an interval of the order of $h/\Delta t$. If a particle crosses a shutter whose opening time has an uncertainty Δt, its energy must be spread over the interval $h/\Delta T$. If the time at which the phase of a light or matter wave takes a given value is known with an uncertainty Δt, then its energy is defined with an uncertainty $h/\Delta t$. In other words measuring with precision the time of an event in quantum physics is paid by an imprecision about the knowledge of the energy of the system. It also means that the more precise we want to measure an energy, the more time it will take.

Einstein's challenge to the time-energy Heisenberg relation: the photon box thought experiment

Einstein: Imagine a box with perfectly reflecting walls in which a few photons are trapped. The box is suspended to a spring in the gravitational field of the Earth so that, by weighing it, one can determine its content of electromagnetic energy via the mass-energy and equivalence principle of general relativity. A precise clock in the box activates a shutter letting a small number of photons to escape. The weight of the box can be measured during a time as long as it takes to achieve an arbitrary precision, before and after the shutter opening window. This opening can be as short as the experimenter decides. So the time-energy relation can be overcome!



Bohr: It cannot be true but I need time to think it out!

General relativity saves Heisenberg uncertainty principle!

Call δm the uncertainty of the mass-equivalent change Δm of em energy in the box due to the escape of photons during the time interval t_0 of the shutter opening. Einstein assumed that t_0 could be made as small as wanted by using an arbitrary precise clock (this is a thought experiment!). Bohr showed that there was an unescapable δt_0 uncertainty due to general relativity, a reminder which must have been embarrasing to Einstein!

Bohr's reasoning:

The gravitational force acting on the scale's spring due to the photons escape has an uncertainty:

$$\delta F = g\delta m$$

This force, acting during time t_0 accelerates the box which acquires a momentum with uncertainty:

$$\delta p = \delta F . t_0 = g\delta m . t_0$$

According to the position-momentum Heisenberg uncertainty, this results in a fuzziness of the altitude of the box in the Earth field:

$$\delta z = \hbar / \delta p = \frac{\hbar}{g\delta m . t_0}$$

At this point, General Relativity intervenes: The clock's altitude uncertainty results in a relative uncertainty of t_0

$$\frac{\delta t_0}{t_0} = \frac{g\delta z}{c^2} = \frac{\hbar}{\delta m c^2 t_0}$$ Hence: $\delta m c^2 . \delta t_0 = \hbar$

We neglected here the spring restoring force. This is legitimate if the period of the spring oscillation is very long compared to t_0. The effect of the additional force due to the change of the pull on the spring during t_0 is then negligible compared to Δmg.

Is it strange that GR has to be invoked for the consistancy of quantum Mechanics?... Not really considering the assumptions made for this thought experiment!

Minimum size of atom imposed by uncertainty relations

Consider the Bohr radius of the Hydrogen atom and ask why the electron cannot get closer to the proton by radiating em energy, as it would do according to Maxwell.

Suppose that the electron gets at distance from nucleus r_0 smaller than a_0. Its potential energy decreases as $-e^2/r_0$ but its localization implies that its momentum uncertainty increases as ~~$\hbar$~~$/r_0$ and its kinetic energy becomes at least ~~$\hbar^2$~~$/2mr_0^2$. Hence the total energy:

$$-\frac{e^2}{r_0} + \frac{\hbar^2}{2mr_0^2}$$

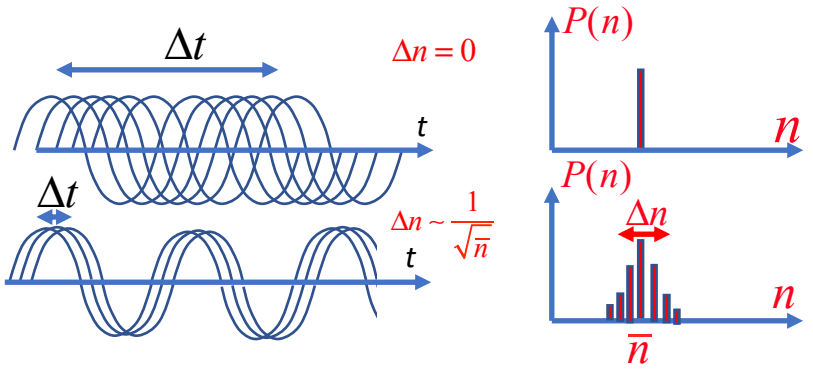
which is minimal for : $r_0 = a_0 = \hbar^2 / me^2$

Same argument explains the zero point energy of harmonic oscillator (see later)

The Heisenberg uncertainy relation prevents the electron to fall on nucleus!

Combined with the Pauli exclusion principle, it explains the size of atoms (electrons must occupy more and more excited orbits as Z increases.)

Uncertainty relation between the amplitude and the phase of a field mode or a harmonic oscillator



$$\Delta E \sim \hbar / \Delta t = \hbar\omega / \Delta\varphi$$

$$\Delta E = \Delta n \hbar\omega \sim \hbar\omega / \Delta\varphi$$

$$\Delta n . \Delta\varphi \sim 1$$

$$\frac{\Delta n}{\bar{n}} \Delta\varphi \sim \frac{1}{\bar{n}}$$

$$\frac{\Delta n}{\bar{n}} = \Delta\varphi \sim \frac{1}{\sqrt{\bar{n}}}$$

When its photon number (hence its energy) is well defined, the phase φ of a field mode is completely random. To have a well defined phase, the field must be in a coherent superposition of different photon numbers around a mean value $\bar{n}$. The best approximation of a classical field has its phase and relative photon number uncertainties equal to $1/\sqrt{\bar{n}}$. The extreme phase stability of lasers (for example in gravitational wave antennas) is related to their very large intensity. Same formulas apply to material quantum oscillators (photons replaced by vibration quanta or phonons).

The principles of quantum physics

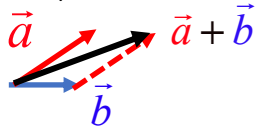
In the first part of this lecture we have presented the conceptual ideas of quantum physics in qualitative terms. We will now present briefly the mathematical framework which has allowed physicists to make quantitative calculations and predictions about quantum phenomena. This framework has emerged during the period 1925-1930 and has expressed by precise mathematical equations what Bohr had semi-intuitively stated with his concept of complementarity.

We will recall the Dirac formalism of quantum physics which describes quantum states as vectors of an abstract Hilbert space and physical observables as Hermitian operators acting on these vectors. The postulates of quantum measurement will then be enunciated. The position, momentum and energy operators of a particle will be described as the generators of the translations in momentum, space and time of the quantum states. This approach gives a deeper meaning to Schrödinger's equation and allows us to re-analyse quantum interference experiments and complementarity in quantitative terms.

Reminder about the rules of real vector spaces

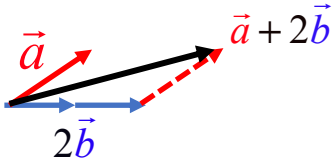
Vectors belonging to a vector space are mathematical objects which may be added and multiplied by real numbers according to distributive and commutative rules. An example is given by the 3D vectors of ordinary euclidian space (vectors representing position, velocity or forces). The vector space may have 2 dimensions (vectors in plane), 3D (vectors in space), 4D (vectors in space-time) or more dimensions…A few rules of vectors addition and multiplication by real numbers are recalled below:

Addition of vectors:



Multiplication by real numbers:

Linear combinations



Scalar product of vectors: commutative application of a couple of vectors on real numbers:

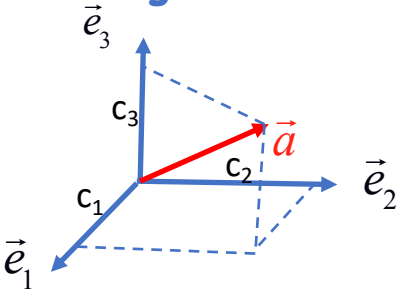
$$(\vec{a},\vec{b}) \rightarrow \vec{a}.\vec{b} = \vec{b}.\vec{a}$$

Distibutivity of scalar product $\alpha\vec{a}.(\beta\vec{b}+\gamma\vec{c}) = \alpha\beta\vec{a}.\vec{b}+\alpha\gamma\vec{a}.\vec{c}$ α,β,γ *...real numbers*

Vector representation in orthogonal basis

Definition of orthonormalize basis of vectors:

$$\vec{e}_i.\vec{e}_j = \delta_{ij} \qquad i = 1,2\cdots d$$



Example of 3D vector space

Coordinates of a vector in a basis:

$$\vec{a} = \sum_{1\le i\le d} (\vec{a}.\vec{e}_i)\vec{e}_i \qquad \vec{a} = \sum_{1\le i\le d} (\vec{a}.\vec{e}_i)\vec{e}_i = \sum_i c_i\vec{e}_i$$

$$c_i = \vec{a}.\vec{e}_i : \textit{real coordinate of } \vec{a} \textit{ in } \{\vec{e}_i\} \textit{ basis}$$

Linear operations on vectors: example of rotations:

The c'_j coordinates of the rotated vector are linear combinations of the c_i's whose coefficients are given by a d x d matrix R_{ij}.

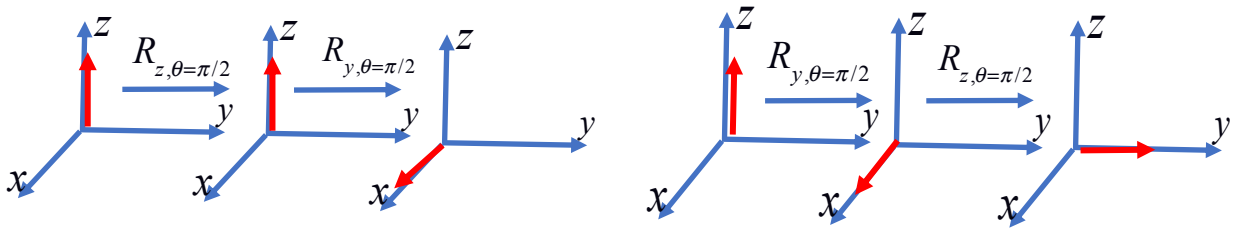
$$R(\vec{a}) = \sum_i (\vec{a}.\vec{e}_i)R(\vec{e}_i) \textit{ with } R(\vec{e}_i) = \sum_j R_{ij}\vec{e}_j \qquad R(\vec{a}) = \sum_j c'_j\vec{e}_j \qquad c'_j = \sum_i R_{ij}c_i$$

Commuting and non commuting operations: example of rotations

Rotations around same axis commute:

$$R_{z,\theta_1} \times R_{z,\theta_2} = R_{z,\theta_2} \times R_{z,\theta_1}$$

Rotations around different axis do not commute:



$$R_{y,\theta=\pi/2} \times R_{z,\theta=\pi/2} \neq R_{z,\theta=\pi/2} \times R_{y,\theta=\pi/2}$$

The Hilbert space of quantum states: Dirac bra-kets

The states of a quantum system are described by vectors in an abstract complex vectorial Hilbert space which obey the rules of linear algebra. The dimension d of the Hilbert space can be finite ($D \geq 2$) or infinite. For sake of simplicity we will first consider the case of systems evolving in a Hilbert space of finite dimension and generalize later to the infinite dimension situation.

Following the elegant notation introduced by Dirac, state vectors are noted by « kets »:

$$|\psi\rangle$$

Any linear combination of kets representing different states of the system is a possible state:

$$|\psi\rangle = \sum_i c_i |\varphi_i\rangle$$

where the c_i's *are complex numbers.* This property expresses the superposition principle of quantum physics, analogous to the superposition principle of optics and electromagnetism. The c_i's are called « probability amplitudes ».

To any ket $|\psi\rangle$, is associated a conjugate "bra" $\langle\psi|$:

$$|\psi\rangle \rightarrow \langle\psi|$$

$\langle\psi|$ is a functional which images any ket $|\varphi\rangle$ onto the body of complex numbers:

$$\langle\psi| \text{ applied to } |\varphi\rangle = \text{complex number noted } \langle\psi|\varphi\rangle$$

The c-number $\langle\psi|\varphi\rangle$ is analogous to the scalar product of two vectors in an ordinary vectorial space. The difference is that the inner product (which is also called the Hermitian product of the two kets) is *a complex number* whose physical meaning will be discussed later.

Hermitian products and projections of quantum states

The Hermitian product of two states is non-commutative:

$$\langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle^*$$

where the star denotes the complex conjugation:

$$(a+ib)^* = a-ib \quad (a,b\ reals)$$

It follows that the correspondence between kets and bras is antilinear:

$$c_1|\psi_1\rangle + c_2|\psi_2\rangle \rightarrow c_1^*\langle\psi_1| + c_2^*\langle\psi_2|$$

In analogy with ordinary vector algebra, two states are orthogonal if:

$$\langle\psi|\varphi\rangle = 0$$

And a state is normalized to unity if:

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

The projection of state $|\Psi\rangle$ on state $|\varphi_i\rangle$ is defined as:

$$|\varphi_i\rangle\langle\varphi_i|\psi\rangle$$

It is the state $|\varphi_i\rangle$ multiplied by the c-number $\langle\varphi_i|\psi\rangle$. This notation lead us to define the projection operator as:

$$P_i = |\varphi_i\rangle\langle\varphi_i|$$

P_i is a linear operator of the Hilbert space transforming any state into a state colinear with $|\varphi_i\rangle$ (analogous to the projection on a vector basis in a real vector space).

In an Hilbert space of dimension d one can define a set of d states forming an orthonormal basis on which any state of the space can be developped (see next slide)

States and operators representations

In a Hilbert space of dimension d, we can define a set of d orthonormalized vectors satisfyng the conditions:

$$\langle\varphi_i|\varphi_j\rangle = \delta_{ij}$$

The sum of the projectors on the $|\varphi_i\rangle$'s is equal to the identity:

$$\sum_i P_i = \sum_i |\varphi_i\rangle\langle\varphi_i| = I \quad (I = identity\ operator)$$

The $|\varphi_i\rangle$ form a complete basis since any state can be developped along it according to:

$$|\psi\rangle = I|\psi\rangle = \sum_i |\varphi_i\rangle\langle\varphi_i|\psi\rangle =$$

$$\sum_i c_i|\varphi_i\rangle \quad (c_i = \langle\varphi_i|\psi\rangle)$$

An operator A in the Hilbert space is a linear application which images any state into another one. The Dirac notation allows us to represent any operator A as=

$$\hat{A} = I \times \hat{A} \times I = \sum_{i,j} |i\rangle\langle i|A|j\rangle\langle j| = \sum_{ij} A_{ij}|i\rangle\langle j|$$

to simplify the notation, I have replaced the notation $|\varphi_i\rangle$ simply by $|i\rangle$. The A_{ij}'s are the matrix elements of the operator A in the basis $|i\rangle$.

$$\hat{A}|\psi\rangle = \sum_{i,j} A_{ij}|i\rangle\langle j|\psi\rangle = \sum_i c_i|i\rangle$$

$$with\ c_i = \sum_j A_{ij}\langle j|\psi\rangle$$

We retrieve here very simply with the Dirac notations the usual rule of matrix algebra.

Eigenstates and eigenvalues of Hermitian operators

An eigenstate of an operator A is a state which is transformed in a colinear state by the action of A:

$$A|a\rangle = \lambda_a |a\rangle$$

The coefficient λ_a is called the eigenvalue of the eigenstate $|a\rangle$.

The adjoint $O^\dagger$ of an operator O is its transpose conjugate, whose matrix elements are in all bases related to those of O by the relation:

$$O^\dagger{}_{ij} = O^*_{ji}$$

Physical observables of a quantum system are associated with Hermitian operators which are their self-adjoint, satisfying the condition:

$$O = O^\dagger \quad \text{hence:} \quad O_{ij} = O^*_{ji}$$

There is a basis in which these observables are diagonal, with real matrix elements $[a_i]$ which constitute the spectrum of the observable:

$$O|i_\alpha\rangle = a_i |i_\alpha\rangle \; and \; O = \sum_{i,\alpha} a_i |i_\alpha\rangle\langle i_\alpha|$$

$$\left[a_i = O_{i\alpha,i\alpha} : real\ eigenvalue \right]$$

The a_i eigenvalue may be degenerate, the eigen-subspace being spanned by several basis states $|i_\alpha\rangle$.

The measurement postulates

When a measurement of the observable O is performed on the system in state $|\psi\rangle$, the result is one of the eigenvalues of the observable. The probability to find a_i is:

$$\Pi_i = \sum_\alpha \langle\psi|i_\alpha\rangle\langle i_\alpha|\psi\rangle = \sum_\alpha |\langle i_\alpha|\psi\rangle|^2$$

(hence the name of probability amplitude given to the Hermitian products of states). We assume here that the state $|\psi\rangle$ is normalized to unity, so that the sum of the Π_i is equal to 1:

$$\sum_i \Pi_i = \langle\psi|\psi\rangle = 1$$

Immediately after the measurement the state of A is projected onto the i^{th} subspace:

$$|\psi_i\rangle = \sum_\alpha |i_\alpha\rangle\langle i_\alpha|\psi\rangle$$

All information is lost about the amplitudes $\langle j|\psi\rangle$ of the initial state with $j \neq i$

This is the measurement induced « collapse » of the state. If the measurement is immediately repeated, the same result is found, the state being then unchanged.

Quantum interferences: if $|\psi\rangle$ is a superposition:

$$|\psi\rangle = \sum_j c_j |\psi_j\rangle \longrightarrow \Pi_i = \sum_\alpha \sum_{j,j'} c^*_j c_{j'} \langle\psi_j|i_\alpha\rangle\langle i_\alpha|\psi_{j'}\rangle$$

The c_j probability amplitudes of state components non-orthogonal to the eigensubspace selected by measurement interfere ($c_j c^*_{j'}$ terms).

Observable mean value: Repeating the measurement of an observable O on an ensemble of systems *prepared in the same quantum state* $|\psi\rangle$ yields a mean value:

$$\langle a_i \rangle = \prod_{i,\alpha} \langle\psi|i_\alpha\rangle a_i \langle i_\alpha|\psi\rangle = \langle\psi|O|\psi\rangle$$

There is a mean square root deviation around this mean value describing the uncertainty of the measurement (see below).

Properties of commuting observables

Consider two commuting observable A and B such that:

$$AB - BA = 0$$

Applying AB and BA on an eigenstate $|i_\alpha\rangle$ of A with eigenvalue a_i we get:

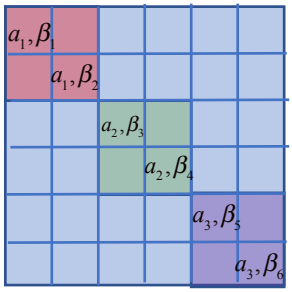
$$BA|i_\alpha\rangle = a_i B|i_\alpha\rangle = A\left[B|i_\alpha\rangle\right]$$

which shows that $B|i_\alpha\rangle$ belongs to the eigensubspace of the eigenvalue a_i of A. B has thus no matrix elements between different eigensubspaces of A. By a change of basis, it is possible to diagonalize B in each eigensubspace of A, yielding:

$$A|\beta_i\rangle = a_i|\beta_i\rangle \quad ; \quad B|\beta_i\rangle = \beta_i|\beta_i\rangle$$

where the $|\beta_i\rangle$ are linear superpositions of the $|i_\alpha\rangle$'s. If the $\{a_i, \beta_i\}$'s do not completely specify the common eigenstate, a third observable C commuting with A and B can be added…etc…until all bases states are unambigously determined.

We define in this way a complete set of commuting observables (CSCO) with a common basis of eigenstates. Each of these states is uniquely defined by the sequence of quantum numbers $[a_i, \beta_i, \gamma_{i\beta}\ldots]$. It could be theoretically prepared (randomly) by performing a measurement of the CSCO's giving as results the corresponding eigenvalues.



Example: A has three eigenvalues each of them being two times degenerate: B has non zero matrix elements only within the three colored boxes. By changing bases, B can be diagonalized in each box, leading to 6 uniquely defined diagonal states.

Measurement of non-commuting observables and uncertainty relations

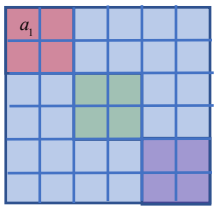
Suppose that one prepares a system in state $|\psi\rangle$ and mesure succcessively observable A and B, then A again. If A and B commute, the second measurement leaves the system in the eigenspace corresponding to the eigenvalue a_i obtained in the first measurement and the subsequent measurement of A yields the same result as the first. Measuring B does not alter the measurement of A and conversely, measuring A does not change the result obtained when measuring B. The observables A and B are said to be compatible

The situation is different if A and B do not commute:

$$AB - BA = \left[A, B\right] \neq 0$$

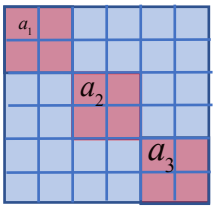
In this case, measuring B projects the system into a state presenting components outside the eigensubspace of A resulting from the first measurement and there is a probability that the repeated measurement of A yield a different result than the first one

After Measuring A



Measurement selects one eigenspace of A (in red)

After measuring B



Measuring B mixes different eigensubspaces of A

Measuring B perturbs the probability distribution of results of measurement of A. The Heisenberg uncertainty relation between x and p is an example of the incompatibility of measuring with arbitrary precision non-commuting observables (see below).

Position, momentum and Hamiltonian operators in x,p bases

We now apply the postulates to the position and momentum operators X and P_x of a particle. We restrict the formulas to one spatial dimension and will extend them to x,y,z when needed. The spectra of X and P_x being continuous, the Hilbert space of the particle is of infinite dimension and the discrete expansions of the states and operators become integrals:

$$\int |x\rangle\langle x| dx = I \quad ; \quad \langle x|x'\rangle = \delta(x-x')$$

$$X|x\rangle = x|x\rangle ; \quad |\psi\rangle = \int |x\rangle\langle x|\psi\rangle dx = \int \psi(x)|x\rangle dx$$

The wave function ψ(x) is the Hermitian product of the bra <x| with the ket |ψ>. The probability to find x between x and x+dx is:

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

The action of X (or a function U(X)) on the wave function amounts to multiplication by x (or U(x)):

$$\langle x|X|\psi\rangle = x\langle x|\psi\rangle = x\psi(x) \quad \langle x|U(X)|\psi\rangle = U(x)\psi(x)$$

Similar formulas apply to the momentum:

$$P|p\rangle = p|p\rangle \quad ; \quad |\psi\rangle = \int |p\rangle\langle p|\psi\rangle dp = \int \tilde{\psi}(p)|p\rangle dp$$

|ψ> is represented by the momentum function $\tilde{\psi}(p)$ = <p|ψ> in the |p> basis, with the Fourier transform (FT) correspondence:

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int \langle p|x\rangle\langle x|\psi\rangle dx = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-ipx/\hbar}\psi(x)dx$$

The wave function of the state $P_x|\psi\rangle$ is obtained in the same way:

$$\langle x|P|\psi\rangle = \int e^{ipx/\hbar} p\tilde{\psi}(p)dp = \frac{\hbar}{i}\frac{\partial\psi(x)}{\partial x}$$

(the FT of the derivative of a function of x is equal to the FT of the function multiplied by the conjugate variable p).

Commutator of X and P_x and standard form of Heisenberg relations

Commutators of X and P components

$$\langle x|[X,P_x]|\psi\rangle = \langle x|[XP_x - P_xX]|\psi\rangle = \frac{\hbar}{i}\left[x\frac{\partial\psi(x)}{\partial x} - \frac{\partial[x\psi(x)]}{\partial x}\right] = i\hbar\psi(x)$$

$$[X,P_x] = [Y,P_y] = [Z,P_z] = i\hbar \times I \qquad [R_i,P_j] = i\hbar\delta_{ij} \times I$$

Standard deviations of X an P:

$$X' = X - \langle X\rangle I \quad ; \quad P'_x = P_x - \langle P_x\rangle \quad \langle X'^2\rangle = \Delta x^2 \quad ; \quad \langle P_x'^2\rangle = \Delta p^2$$

For any ket |ψ> consider the ket (λ real): $|\Psi\rangle = (X' - i\lambda P'_x)|\psi\rangle$

and compute its norm:

$$\langle\Psi|\Psi\rangle = \langle\psi|(X' - i\lambda P'_x)(X' + i\lambda P'_x)|\psi\rangle$$

$$\langle\Psi|\Psi\rangle = \langle\psi|X'^2 + \lambda^2 P'^2_x + i\lambda(X'P'_x - P'_xX')|\psi\rangle$$

$$\langle\Psi|\Psi\rangle = \Delta x^2 + \lambda^2\Delta p_x^2 - \lambda\hbar \geq 0 \quad (\forall\lambda \text{ real})$$

Norm always positive requires that equation has no real racines , hence:

$$\hbar^2 - 4\Delta x^2\Delta p_x^2 \leq 0 \quad \rightarrow \quad \boxed{\Delta x\Delta p_x \geq \frac{\hbar}{2}}$$

Apply to the ground state of a Harmonic oscillator. The mean energy of the oscillator, sum of its kinetic and potential contributions is:

$$\langle p^2\rangle/2m + m\omega^2\langle x^2\rangle/2$$

Ground state energy obtained by replacing $\langle p^2\rangle = \Delta p^2$ by $\hbar^2/4\langle x^2\rangle$ and minimizing with respect to $\langle x^2\rangle$:

$$\langle x^2\rangle_{min} = \hbar/2m\omega ; \langle p^2\rangle_{min} = \hbar m\omega/2$$

The potential and kinetic energy of ground state are both equal to ħω/4 and total energy to ħω/2 Due to X and P_x non commutation oscillator has zero point quantum fluctuations preventing it to be motionless.

The Hamitonian as the energy operator in Hilbert space

The Hamiltonian H = $P^2/2m$ + U(x) of a particle, is its energy observable. In the x-representation the action of H on the wave function writes:

$$\langle x|H|\psi\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\psi(x)$$

The eigenstates of the Hamitonian are the energy states of the particle. They satisfy the eigenvalue equation:

$$H|\psi\rangle = E|\psi\rangle$$

which in the 3D X,Y,Z-representation is a second order differential equation for the wave function:

$$-\frac{\hbar^2}{2m}\Delta\psi(\vec{r}) + U(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

This is the so-called « time-independent » Schrödinger equation. It has exact solutions for two problems:

The hydrogen atom:

$$U(\vec{r}) = -\frac{e^2}{r} \quad \rightarrow \quad E_{n,l,m} = -\frac{me^4}{2\hbar^2}\frac{1}{n^2} \quad (n = 1,2....\infty)$$

Schödinger equation gives the same spectrum as Bohr model. H commuting with the square of angular momentum L^2 and its component along Oz, L_z, the energy levels are degenerate, hence the quantum numbers *l* and *m* labelling the states in addition to energy (see lecture 6).

The harmonic oscillator of angular frequency ω:

$$U(\vec{r}) = \frac{m\omega^2 r^2}{2} \quad \rightarrow \quad E_{n_x,n_y,n_z} = (n_x + n_y + n_z + 3/2)\hbar\omega$$

Each degree of freedom (x,y,z) is a 1D harmonic oscillator with spectrum: $E_n = (n + \frac{1}{2})\hbar\omega$

Translation of quantum state in time, position & momentum

We now show that the complex exponentials of H,P and X are the translation operators in time, space and momentum of quantum states

A function f(O) of an observable O is defined by its action on a basis of O (with eigenvalues a_i) as:

$$f(O)|i_\alpha\rangle = f(a_i)|i_\alpha\rangle$$

and the action of f(O) on state |ψ> writes:

$$f(O)|\psi\rangle = \sum_{i,\alpha} f(a_i)|i_\alpha\rangle\langle i_\alpha|\psi\rangle$$

Applying this definition to the Hamiltonian H, we get:

$$e^{-iHt/\hbar}|\psi(0)\rangle = \sum_{E,\alpha} e^{-iEt/\hbar}|E,\alpha\rangle\langle E,\alpha|\psi(0)\rangle = |\psi(t)\rangle$$

The complex exponential of the Hamiltonian operator:

$$U(t) = e^{-iHt/\hbar}$$

describes the translation in time of the quantum states:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

Consider now the complex exponential of the momentum operator P_x

$$T_{x_0}(P) = \exp(-ix_0 P/\hbar)$$

we get:

$$\langle x|e^{-iPx_0/\hbar}|\psi\rangle = \int dp e^{-ipx_0/\hbar}\langle x|p\rangle\langle p|\psi\rangle =$$

$$\frac{1}{\sqrt{2\pi\hbar}}\int dp e^{ip(x-x_0)/\hbar}\tilde{\psi}(p) = \psi(x - x_0)$$

The momentum operator generates the translation in space of the quantum state.

In a symmetrical way the operator:

$$T_{p_0}(X) = \exp(ip_0 X/\hbar)$$

translates the quantum state momentum:

$$\langle p|\exp(ip_0 X/\hbar)|\psi\rangle = \tilde{\psi}(p - p_0)$$

The position operator is the generator of the translations in momentum space.

Concluding remarks

The formalism of quantum physics has emerged in 1925, shortly after de Broglie hypothesis of matter waves, with the discovery of Schrödinger's equation and of an equivalent formulation by Heisenberg who had developed a matrix description of physical obervables. The concepts of complementarity and of uncertainties in the measurement of incompatible physical quantities, first discussed qualitatively by Bohr was given a rigorous mathematical basis when the Hilbert space formalism of quantum theory has been discovered. This theory is essentially probabilistic as opposed to the absolute determinism of classical physics.

The quantum states of a physical system are vectors in an abstract Hilbert space, obeying to a linear algebra. The inner products of two vectors in this space are c-numbers. Any physical obervable is associated to a Hermitian operator in the Hilbert space whose eigenstates form a basis on which any state can be developed. When measuring an obervable on a system in a given quantum state, one obtains randomly one of the eigenvalues of the observable spectrum and the state is irreversibly projected onto the corresponding eigensubspace. The probability of the outcome is the square of the norm of this projection. If the measured state is a superposition of several states non orthogonal to the eigenspace corresponding to the result, the complex amplitudes of this superposition interfere in the outcome probability. The measurement perturbs in an irreversible way the observed system's state, making it impossible to determine with precision the values of observables described by non-commuting operators. We will continue to discuss the basic concepts of the quantum theory and their physical implications in lectures 6 and 7.