

M2 course notes
Microlocal Analysis
 (by C. Cheverry)

Sessions about quantum mechanics

Chapter 1 on

The **Stone-Von Neumann** theorem

(physical motivations, statement and ideas of proof)

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0. INTRODUCTION

We give the context of the discussion, the objectives and the motivations. We also produce a rapid historical overview.

0.1. Context. In quantum mechanics, physical observables (that is the mesurable quantities) are represented by linear operators on Hilbert spaces denoted by \mathcal{H} (describing the states of the system). This is in particular the case of the *position* operator Q and of the *momentum* operator P . For experimental and historical reasons (that we will recall), these operators must satisfy the following canonical commutation relations:

$$(CCR) \quad [Q, P] = QP - PQ = i\hbar Id \quad \text{where } \hbar \sim 10^{-34} \text{ is the reduced Planck constant.}$$

0.2. Purpose. To better understand the mathematical foundations of quantum mechanics by classifying all the triplets (\mathcal{H}, Q, P) leading to (CCR) .

0.3. Motivations. The electromagnetic radiation including the visible light (which occupies a very small part of the electromagnetic spectrum, namely wavelengths between 400 and 800 nm) has always fascinated physicists and numerous mathematicians. It makes life on Earth possible (through the photosynthesis); it is also at the origin of almost all power sources ; and it gives rise to numerous applications: the fire, heating source during prehistory, is a first example whereas health and communications are more recent illustrations. On the scientific side, it is one of the more complex and mysterious phenomenon. It contributed to a number of scientific revolutions, and likely will be again in the future. There is a common understanding that electromagnetic radiation has the properties of waves (at large scales) but its microscopic behavior also implies corpuscular facets (notion of photon). To start with, it is important to keep in mind some historical landmarks on the different conceptions of light.

0.4. Historical landmarks. The concept of light has a long history behind it.

0.4.1. Period before 1900. This is called the *classical* period. We highlight below some major benchmarks:

- Euclid's Optics from Euclide (300 av. J.-C.);
- the Book of Optics from Ibn Al-Haytham (965). Up to middle age, it was thought that the eyes were being created some light which were coming to illuminate the objects. It was not until the 1000s that the arab scientific Ibn Al-Haytham undermines this theory. He showed by means of experiment that the eyes are optical instruments instead of being generators of light.
- the world from R. Descartes (1596), this is a position statement for heliocentrism (against geocentrism);
- the Treatise on Light from C. Huyghens (1629), wave theory;
- the Opticks from I. Newton (1642), corpuscular theory (grain of light);
- Return to the wave theory with T. Young (1773, polarisation of light), A. Fresnel (1788, discovery of infrared and ultraviolet rays), J.-C. Maxwell (1831, finding of Maxwell equations for the propagation of electromagnetic waves), H. Lorentz (1853, luminiferous aether), H. Poincaré (1854, works about the speed of light), A. Einstein (1879, relativity).

The interaction between the matter (in the form of plasma) and electromagnetic waves can be described at large scales (... , tokamaks, magnetospheres, planetary systems, galaxies, ...) by quasilinear hyperbolic systems which are built with the equation of A. A. Vlasov (1908-1975) and the equations of J. C. Maxwell (1831-1879). The mathematical understanding of this system requires some analysis of partial differential equations as well as notions coming from the worlds of pseudo-differential operators and nonlinear analysis.

0.4.2. Period after 1900. This is the *quantum revolution*. It is based on two principles:

- The equivalence between mass and energy:
 - $E^2 = p^2c^2 + m^2c^4$ for a particle of momentum p and proper mass m , which becomes $E = mc^2$ for a particle at rest ($p = 0$) in a Galilean reference frame;
 - For a photon (which has zero mass and speed c in all inertial frames - it is never at rest), we set $E = pc$ (De Broglie relation) and $E = h\nu$ (relation of Planck-Einstein where $h \sim 6 \times 10^{-34}$ is the Planck constant and ν is the radiation frequency).
- The duality between the two behaviors:
 - corpuscular: description through quanta (or photons with energy $E = h\nu$). The equations of propagation are those of Heisenberg (they have been written during the year 1925);
 - waves: description through the probability of the presence of particles. The equations of propagation are those of Schrödinger (they have been written during the year 1926).

The synthesis between these two representation modes (corpuscular with Heisenberg and waves with Schrödinger) is achieved through the [Stone-Von Neumann theorem](#) (1931) which is presented in this text.

1. BASIC PRINCIPLES OF QUANTUM MECHANICS

We provide here some benchmarks (see the chapter 1 of this [text](#)) about the experiments and the physical ideas that have led to the statement of the [Stone-Von Neumann theorem](#). In this first part, the result is given without proof. The purpose is first to motivate the approach of Von Neumann, to put it in its historical context, and to better situate it at the interface with physics. The reader who is interested by further mathematical developments may find in [7,8,9] other avenues for reflection as well as extra references.

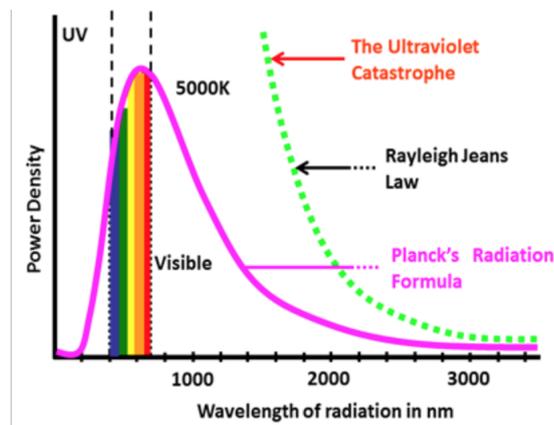
1.1. **The Black-body radiation.** Works of [M. Planck](#) (born in 1858).

[Planck's law](#) describes the repartition of electromagnetic energy (which is proportional to the density of photons) radiated by a black body at thermal equilibrium (that is with a given temperature) in terms of the wave length (which is inversely proportional to the energy of a photon). The [ultraviolet catastrophe](#) is the expression used by the austrian physicist P. Ehrenfest to designate the results of the first experiences which (in the range of high frequencies) were in contradiction with the conclusions of classical physics (see the [Wien's displacement law](#) and the [Rayleigh-Jeans law](#)).

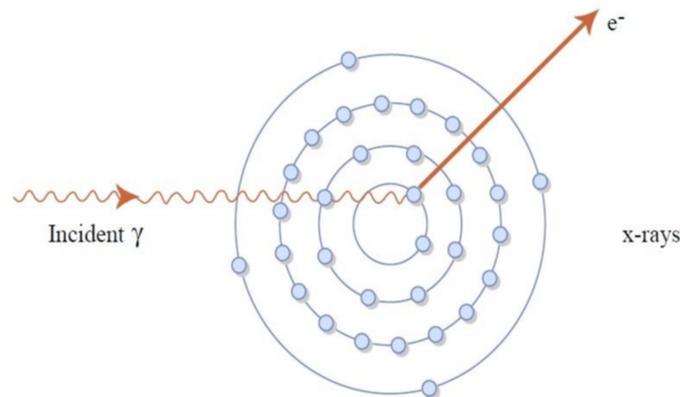
TABLEAU 1. The black-body radiation

black body	temperature (K or C°)	radiation (hz)	intensity (Cd)
black hole	~ 0	~ 0	~ 0
iron bar	10°	infrared (grey)	1
iron bar	100°	red/yellow	2
iron bar	1000°	white	4
sun	5000°	ultraviolet	catastrophe !

[Planck's law](#) addresses the [ultraviolet catastrophe](#) noted above. In the range of high frequencies, it provides more precise and reliable forecasts than the preceding ones. To deduce it from fundamental principles, M. Planck takes the view that heated materials can be described by a set of oscillators implying discrete exchanges of energy. This quantum of action $\Delta E = h\nu$ measures the granularity of energetic exchanges. At that time, the formula of Planck was considered as a mathematical trick (the light was still seen as a wave).



1.2. **The photoelectric effect.** Works of **A. Einstein** (1879-1955) which was rewarded with the nobel prize (1921).



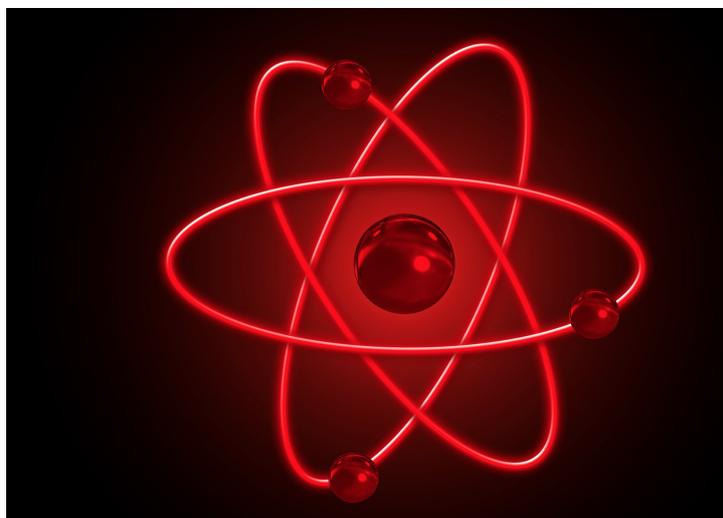
A metal plate is illuminated by electromagnetic waves having a given amplitude and a fixed frequency ν . We find that electrons coming from the atoms can be emitted but this phenomenon does not occur when the incident frequency is too much small, when it is below some threshold. This effect is not impacted by the amplitude (which counts the number of implicated photons) of the wave, whether it is large or not.

The explanation is as follows. The light may be viewed as a set of elementary particles called photons, having each a discrete quantity of energy $E = h\nu$. Each photon interact with an atom. The electron can leave the metal surface when the incident photon has a sufficient energy E , above the **exit work** W (which maintains the electron near its atom). On the other hand, the amplitude does not play a role in this mechanism (which does not depend on the number of photons implied).

When the light beam is composed with photons having a frequency below the threshold frequency, contrary to preceding theories, the uprooting of electrons does not happen. The increase of the amplitude implies indeed that the received energy has increased. But the accumulation is handled differently. The energy of low frequency photons is first absorbed by the atom and then it is re-radiated in the form of photons (with possibly new frequencies and thereby change of colors) and not in the form of photoelectrons.

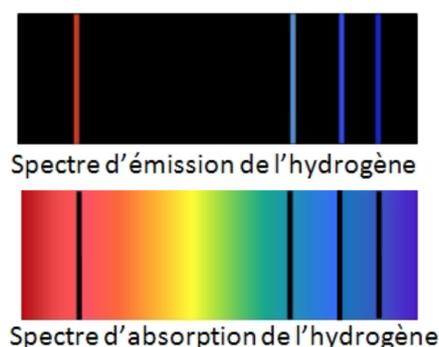
The above photoelectric effect has produced the first experimental evidence that electromagnetic radiation is intrinsically made of grains of energy $h\nu$. The **photon** of frequency ν was born !

1.3. **The Bohr model.** Works of **N. Bohr** (born in 1885).



N. Bohr (and his colleagues) have questioned the atomic structure of the **hydrogen** (isotope ^1H : one proton and two electrons). His theory which has become obsolete was established on a **planetary model** (developed earlier by Rutherford) for the motion of electrons around the nucleus (there are similarities with the moon turning around the earth - except that the electromagnetic force comes to replace the gravitation force).

However, from Maxwell's law, an electron submitted to an acceleration should continuously emit some electromagnetic radiation. It should follow a concentric spiral (and not a circle) and subsequently crash into the nucleus (in about one nanosecond). These two aspects (fall and emission of radiations) are in contradiction with the observations. Indeed, we see that the different **spectral lines** of the hydrogen atom have a discrete repartition.



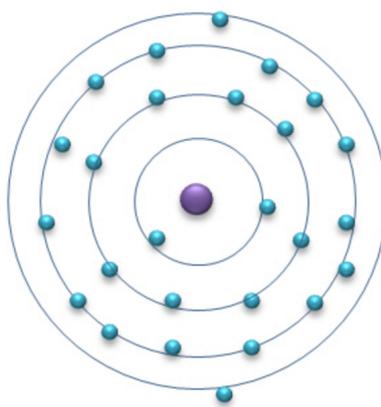
To take into account these observations, N. Bohr postulated that:

- only a finite number of (stationary) orbits are occupied;
- the electron does not radiate or absorb energy except when passing from one orbit to one another.

It follows that:

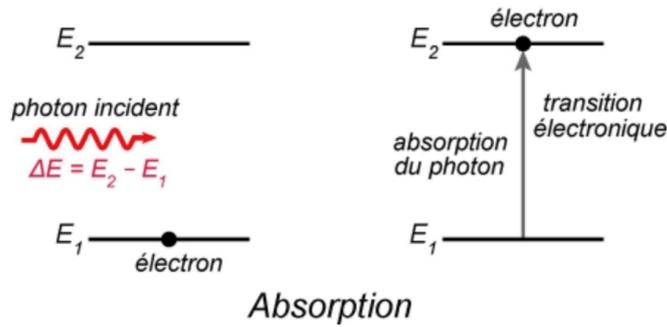
- the energies of the electrons are quantified: $E_n = (-13,6\text{ev})/n^2$ with $n \in \{1, 2, 3, \dots\}$;
- the radii of the orbits are quantified: r_n with $n \in \{1, 2, 3, \dots\}$.

Various possible positions of the electron around its nucleus



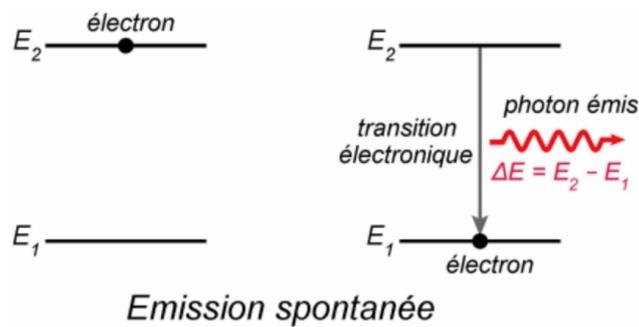
The electrons which turn around the nucleus are said in a **bound state**. Their energy is then negative. The bound state of minimal energy (E_1) is called a **ground state**. This is the only one that is stable. The other (excited) states are unstable. They can transit from one level of energy to another according to the following mechanisms (which among other things may explain the color of the objects):

- *Absorption.* The electron may pass from the state E_n to the state E_m with $m > n$ when a photon of frequency $\nu_{nm} \geq (E_n - E_m)/h$ hits the atom (with some energy input $\Delta E = E_m - E_n$). The case of two energies E_1 and E_2 is described on the picture below:



If the energy $h\nu$ of the photon is enough ($h\nu > -E_n$), the electron located on the n^{iem} layer may leave the atom (with a kinetic energy that absorbs a part of the energy surplus $h\nu + E_n$). The electron is then in some unbound state, and the remaining atom is ionized.

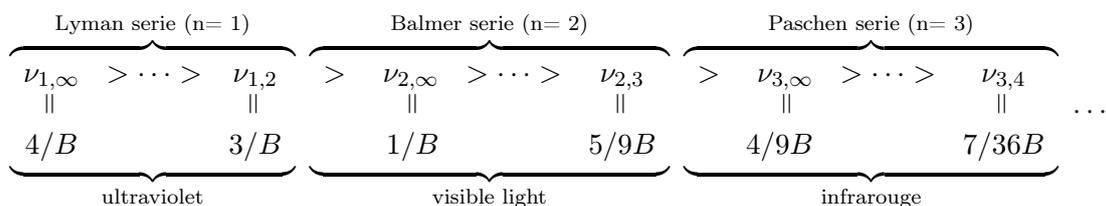
- Spontaneous *emission*. When the electron is in an excited state, it can transit from the state E_m to a state of lower energy E_n with $m > n$. A photon is then emitted, removing the excess of energy $\Delta E = E_m - E_n$. The case of two energies E_1 and E_2 is described on the picture below:

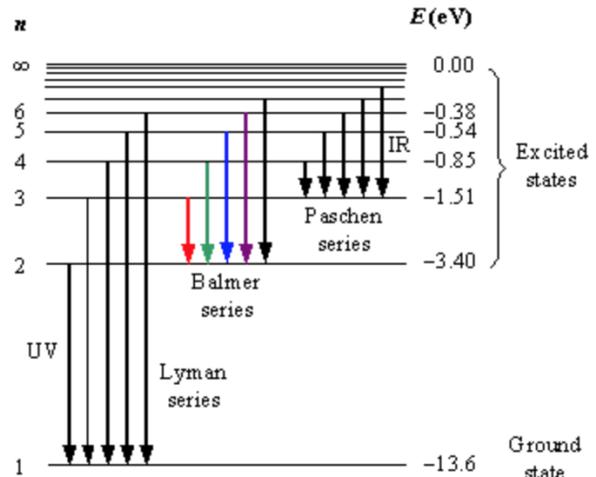
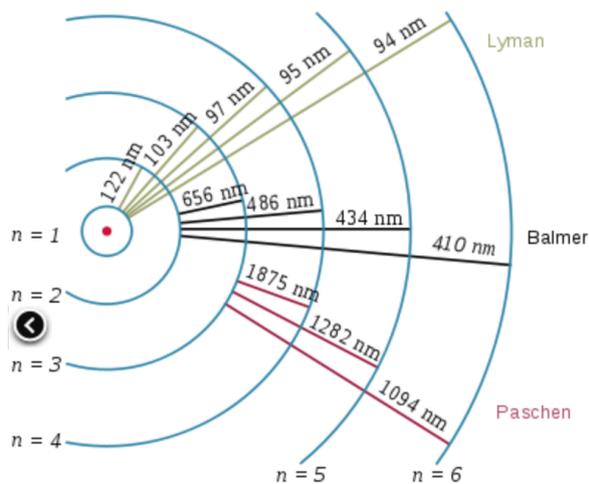


The energies $E_n = (-13,6eV)/n^2$ are adjusted in coherence with the observations concerning the [spectral lines of the hydrogen atom](#). In particular, the [Balmer formula](#) was available. It was then improved into the [Rydberg formula](#):

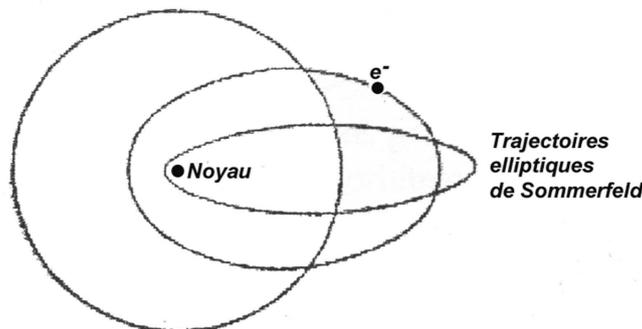
$$\lambda_{nm} = \frac{B}{4} \frac{m^2 n^2}{m^2 - n^2}, \quad \nu_{nm} = \frac{1}{\lambda_{nm}} = \frac{4}{B} \left(\frac{1}{n^2} - \frac{1}{m^2} \right), \quad n < m.$$

The *quantum* frequencies ν_{nm} (so called because they correspond to the gaps observed in the spectral lines) are brought together in "series" (Lyman, Balmer, Paschen, ...):





Remark 1 (The Bohr-Sommerfeld atom). The Bohr model has been (just after 1916) improved by A. Sommerfeld (1868). The goal was to take into account the (very slight) doubling of the spectral lines. To this end, A. Sommerfeld introduced relativistic corrections and he described no more the orbits as circles but instead as ellipses. He used two quantum numbers (say a and b) instead of one (r) in the case of circles. The numbers a and b quantified into a_1, a_2, \dots and b_1, b_2, \dots are associated with the lengths of the large and small axis of ellipses (when r_1, r_2, \dots were associated with the radii of the circles).



The reader can refer to this [text](#) for more details on the Bohr atom, as well as a (brief) quantum description of it.

1.4. Confrontation of the Bohr model with observations. In the Bohr model, the electron is viewed as a "classical" particle whose position $q_n^c(t) \in \mathbb{R}^3$ lies on the n^{th} orbit and which moves periodically along a circle. The function q_n^c can be expanded in a Fourier series according to

$$(1.1) \quad q_n^c(t) = \sum_{\alpha=-\infty}^{+\infty} A(n, \alpha) e^{2\pi i \nu(n,1) \alpha t}, \quad A(n, -\alpha) = \bar{A}(n, \alpha).$$

By this way, two *classical* parameters (called classical because they correspond to a classical representation of the motion of the electron) are:

- the *classical* frequencies $\nu(n, \alpha) := \nu(n, 1)\alpha$;
- The *classical* amplitudes $A(n, \alpha)$.

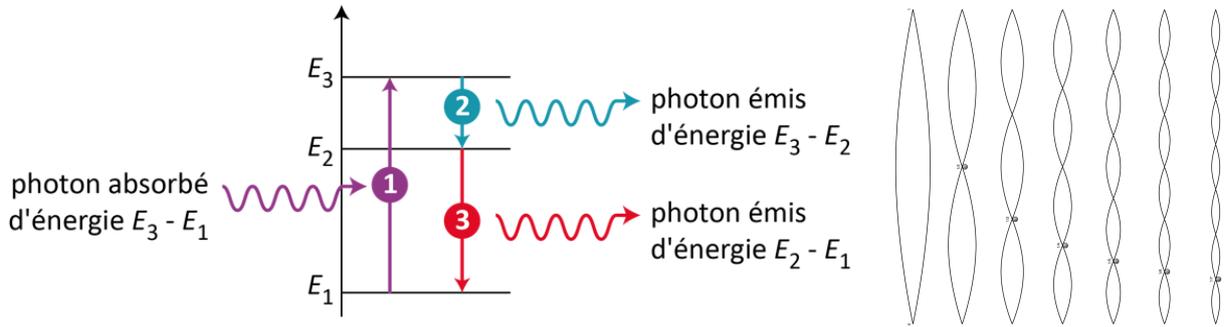
For various reasons, the quantum frequency $\nu_{n(n-\alpha)}$ is linked to the classical frequency $\nu(n, \alpha)$. This comparison can be made for instance at the asymptotic level. Indeed, for α fixed and n which goes to $+\infty$, the Rydberg formula indicates that:

$$\nu_{n(n-\alpha)} = -\frac{8}{Bn^3} \alpha + \mathcal{O}\left(\frac{1}{n^4}\right) \sim \nu(n, 1) \alpha = \nu(n, \alpha) \quad \text{with} \quad \nu(n, 1) = -\frac{8}{Bn^3}.$$

Similarly, the quantum amplitude $A_{n(n-\alpha)}$ (which measures the effective intensity of the spectral line observed at the frequency $\nu_{n(n-\alpha)}$) can be related to the classical amplitude $A(n, \alpha)$. Pushing the analogy to the side of (1.1), we can imagine to describe the movements $q_n^q(t)$ of a quantum electron on the n^{th} orbit according to

$$(1.2) \quad q_n^q(t) = \sum_{\alpha=-\infty}^{+\infty} A_{n(n-\alpha)} e^{2\pi i \nu_{n(n-\alpha)} t}.$$

It is interesting to compare through two pictures the visions underlying the repartition of the quantum and classical frequencies.



The above left drawing highlight the relations:

$$(E_n - E_{n-\alpha'}) + (E_{n-\alpha'} - E_{n-\alpha}) = E_n - E_{n-\alpha}$$

which imply that

$$(1.3) \quad \nu_{n(n-\alpha')} + \nu_{(n-\alpha')(n-\alpha)} = \nu_{n(n-\alpha)}.$$

On the contrary, the above right drawing is inspired by the classical model of vibrating strings for which the frequencies are multiple of a fundamental frequency $\nu(n, 1)$. Since $\nu(n, \alpha) = \nu(n, 1) \alpha$ for all $\alpha \in \mathbb{Z}$, we have:

$$(1.4) \quad \nu(n, \alpha') + \nu(n, \alpha - \alpha') = \nu(n, \alpha).$$

Remark 2 (Comparison of frequency structures). *It is important to retain that the quantum frequencies ν_{n_j} do not satisfy the relations (1.4) but (1.3). We will see that the ν_{n_j} can be interpreted as the eigenvalues of operators. This is why it is so interesting to consider the algebraic and/or geometrical structures revealed by the picture (in \mathbb{R} or \mathbb{C}) of the spectrum. Besides, note that replacing (1.1) by (1.2), we pass from the framework of periodic functions to the one of almost periodic functions, that has been defined during this period (around 1923) by H. Bohr (danish mathematician and footballer, brother of Niels Bohr).*

On the other hand, for α fixed and n large, the relation (1.4) can be used for the $\nu_{n(n-\alpha)}$ with a good degree of approximation. This is in the spirit of Bohr **correspondence principle** which states that at the limit of large quantum numbers (here n) characterizing the atomic systems, we must recover the formula of classical physics.

Remark 3 (A word about semi-classical analysis). *This idea of Bohr on the transition between quantum and classical physics has lead to a branch of mathematics, the semi-classical analysis (for which it is often the parameter h that is chosen as going to zero). The reader can look at this presentation of Y. Colin de Verdière or, for a commented bibliography, to this text of B. Helffer.*

2. THE MATRIX MECHANICS

Matrix mechanics is a formulation of quantum mechanics created by **W. Heisenberg**, Max Born, and Pascual Jordan in 1925. It was the first conceptually autonomous and logically consistent formulation of quantum mechanics. Driven by a sort of **positivism** (but **can we create the world by looking at it?**), W. Heisenberg gets away from the conceptual model of Bohr to retain that the effective amplitudes $Q_{nm}(t) := A_{nm} e^{2\pi i \nu_{nm} t}$ that are extracted from the signal $q_n^q(t)$ and that verify (due to their definition):

$$(2.1) \quad i \hbar \frac{d}{dt} Q_{nm}(t) = (E_m - E_n) Q_{nm}(t), \quad \hbar = \frac{h}{2\pi}.$$

2.1. The Copenhagen interpretation. The school of Copenhagen was an intellectual current which considers that that it does not make sense to talk about objects without measuring them. It was initiated by N. Bohr, W. Heisenberg, **P. Jordan** and **M. Born** who decided to focus on the observable quantities which are the $Q_{nm}(t)$ and the E_n , and to cross-tabulate them:

$$Q(t) = \begin{pmatrix} Q_{11}(t) & Q_{12}(t) & \cdots & Q_{1n}(t) & \cdots \\ Q_{21}(t) & \ddots & & & \\ \vdots & & \ddots & & \\ Q_{n1}(t) & & & & \\ \vdots & & & & \end{pmatrix}, \quad H = \begin{pmatrix} E_1 & 0 & \cdots & 0 & \cdots \\ 0 & E_2 & & & \\ \vdots & & \ddots & & \\ 0 & & & & \\ \vdots & & & & \end{pmatrix}.$$

The **observables** are the infinite matrices $Q(t)$ and H which can be viewed as acting on the state space which is made of the **states** built with the vectors of $\mathbb{C}^{\mathbb{N}}$ (those are the elements of a complex separable Hilbert space). The operator $Q(t)$ is called **position operator** because it combines the effects of the $q_n^q(t)$ into a complete signal

$$(2.2) \quad q^q(t) = \sum_{n \in \mathbb{Z}} q_n^q(t) = \sum_{n,m} A_{nm} e^{2\pi i \nu_{nm} t}.$$

The function q^q must be real valued. This means that $A_{mn} = \bar{A}_{nm}$. From its definition and from the matrix rules of computation, the observable $Q(t)$ evolves in time according to the *Heisenberg equation*:

$$(2.3) \quad i \hbar \frac{d}{dt} Q = [Q, H], \quad [Q, H] := QH - HQ.$$

The observable H that is constant in time and that commutes with itself must also satisfy (2.3). Besides, by analogy with the classical situation, we can deduce from (1.2) a quantum momentum, or impulsion, denoted by $p_n^q(t)$ and given by:

$$(2.4) \quad p_n^q(t) = m \frac{d}{dt} q_n^q(t) = \sum_{\alpha=-\infty}^{+\infty} P_{n(n-\alpha)}(t), \quad P_{nm}(t) := 2\pi i m \nu_{nm} A_{nm} e^{2\pi i \nu_{nm} t}.$$

Again, the coefficients $P_{nm}(t) = \bar{P}_{mn}(t)$ are solutions to (2.1), whereas the resultant observable $P(t) := (P_{nm}(t))_{nm}$ satisfies (2.3). The operator $P(t)$ is called the **momentum operator** because it combines the effects of all the $p_n^q(t)$. Indeed, we can sum on n the $p_n^q(t)$ to recover the observed complete signal $p^q(t)$.

These considerations are the premises of the **mathematical formulations of quantum mechanics** (which were axiomatized by J. Von Neumann in 1932 in his book **Mathematical Foundations of Quantum Mechanics**). They stipulate that:

All observables evolves in time according to the equation (2.3) of Heisenberg.

In classical mechanics, the physical quantities are the energy, the momentum, the **magnetic moment**, ... They can be determined through the positions q and the momentum p . For instance,

for the harmonic oscillator (the spring), the energy is given by the hamiltonian:

$$H(q, p) = \frac{1}{2} (q^2 + p^2).$$

But how can we compute the observable H with the help of the observables Q and P ? By extrapolation, we can think about:

$$H(q^q(t), p^q(t)) = \frac{1}{2} (q^q(t)^2 + p^q(t)^2).$$

In view of the structure (2.2) of the implemented signals, this leads to consider products of the type

$$(2.5) \quad \left(\sum_{n,m} A_{nm} e^{2\pi i \nu_{nm} t} \right) \left(\sum_{p,q} B_{pq} e^{2\pi i \nu_{pq} t} \right) \\ = \sum_{m \neq p} A_{nm} B_{pq} e^{2\pi i (\nu_{nm} + \nu_{pq}) t} + \sum_{n,q} \left(\sum_m A_{nm} B_{mq} \right) e^{2\pi i \nu_{nq} t}$$

where the law (1.3) has been exploited to obtain simplifications. The right hand side is "almost" of the form (2.2), but not completely ...

Remark 4 (Composition rules). *These nonlinear considerations are typical of geometric optics [5]. We observe a sum of the frequencies and a multiplication of the intensities (coefficients). In this process, the relation (1.3) expresses a resonance (correlation of the frequencies). It highlights the amplitude of the coefficients which are on the right of (2.5), that is:*

$$(2.6) \quad (AB)_{nq} = \sum_m A_{nm} B_{mq}.$$

The sum that implies the indices $m \neq p$ (which are not compatible with the preceding writing) are neglected.

The precise reasons which motivated W. Heisenberg towards the composition rules (2.6) (without knowing the matrix composition) are analyzed in [2]. From the above, we can see that the matrix composition is imposed by: *linear* considerations at the level of (2.3) and *non linear* considerations concerning (2.6). The solution of (2.3) is non stationary (and therefore non trivial) when the two observables Q and H do not commute.

In the textbook case provided by the [quantum harmonic oscillator](#) for which

$$H = \frac{1}{2} (Q^2 + P^2) \quad (\text{quantum harmonic oscillator}),$$

to study the source term (2.3), we need to commute Q and P . Supported by N. Bohr, the group comprised of [M. Born](#), [P. Jordan](#) and of W. Heisenberg settle down to work and comes to the conclusion that the position observable Q and the momentum observable P must satisfy the following [canonical commutation relation](#) (CCR in abbreviated form):

$$(2.7) \quad [P, P] = 0, \quad [Q, Q] = 0, \quad [P, Q] = -i\hbar Id.$$

Remark 5. *In space dimension d , the positions and momenta are indexed by $i \in \{1, \dots, d\}$. We work with P_i and Q_i and there are $3d^2$ relations which are:*

$$(2.8) \quad [P_i, P_j] = 0, \quad [Q_i, Q_j] = 0, \quad [P_i, Q_j] = -i\hbar Id \delta_{ij}.$$

This is [P. Dirac](#) who (around 1925) made the link between (2.8) and the relation $\{p, q\} = 1$ which is satisfied in [Hamiltonian mechanics](#) by the [Poisson brackets](#) $\{p, q\}$ implying the classical variables q and p which are canonically conjugate. For a system with d degrees of freedom, the d coordinates q_i of q determine the position of a point q on a differentiable manifold \mathcal{V} with d dimensions. The conjugate momentum p is an element of the cotangent space $T_p^* \mathcal{V}$. The $2d$

coordinates of (q, p) represent a position in the **phase space** $T^*\mathcal{V}$ which is equipped with the **symplectic bilinear form**:

$$\sigma := \sum_{i=1}^d dq_i \wedge dp_i.$$

We say that the transformation $\mathcal{T} : T^*\mathcal{V} \rightarrow T^*\mathcal{V}$ is canonical when it conserves the symplectic structure. Given a function $f : T^*\mathcal{V} \rightarrow T^*\mathcal{V}$, the question is to know how to associate to it (in a natural and coherent way) an operator on $L^2(\mathcal{V})$. This is the problem of the **geometric quantization** (called sometimes canonical) which tries to connect the symplectic manifolds (seen as phase spaces, think about $T^*\mathcal{V}$) and their canonical transformations \mathcal{T} with on the other side the Hilbert spaces \mathcal{H} - think about $L^2(\mathcal{V})$ - and the associated unitary operators $\mathcal{U}(\mathcal{H})$. The passage from the classical physical quantities to the quantum observables must follow the **correspondence principe**. In the case $d = 1$ and $\mathcal{V} \equiv \mathbb{R}$, the basic rules consists in associating to the coordinate q the (unbounded) multiplication operator by $q \times$ and to the coordinate p the (unbounded) derivative operator $-i\hbar\partial_q$. Thus, we have to consider the actions:

$$\begin{aligned} q \times : \mathcal{C}_0^\infty(\mathbb{R}) &\rightarrow L^2(\mathbb{R}) & -i\hbar\partial_q : \mathcal{C}_0^\infty(\mathbb{R}) &\rightarrow L^2(\mathbb{R}) \\ f(q) &\mapsto q \times f(q), & f(q) &\mapsto -i\hbar\partial_q f(q). \end{aligned}$$

More generally, we can retain the table below.

TABLEAU 2. Correspondence between the classical and quantum observables

Physical quantity a	Observable A
Position x, y, z, r	Multiplication by x, y, z, r
Potential energy $V(r)$	Multiplication by $V(r)$
Momenta p_x, p_y, p_z	Derivations $-i\hbar\partial_x, -i\hbar\partial_y, -i\hbar\partial_z$
Momentum vector p	Gradient $-i\hbar\nabla$
Kinetic energy $E_c = p ^2/(2m)$	Laplacien $-\hbar^2\Delta/(2m)$
Total energy $E = E_c + V(r)$	Hamiltonian $-\hbar^2\Delta/(2m) + V(r)$
Orbital kinetic moment $L = r \times p$	$L = -i\hbar r \times \nabla$

Remark 6 (On the list of observables). *There exist quantum observables that are not directly issued from classic observables (which are functions of q and p). This is the case for instance for the **spin** which, like for the mass or the electric charge, expresses some internal property of particles. It follows that the phase space associated with a quantum particle located inside \mathcal{V} is in fact bigger than $L^2(T^*\mathcal{V})$. Typically, it looks like $L^2(T^*\mathcal{V}) \times \mathbb{C}^n$ for some $n \in \mathbb{N}^*$.*

*The spin is often assimilated to some intrinsic kinetic moment. It is also sometimes associated to notions of **polarization** and of **helicity** that are derived from it. It can also be obtained by geometrical considerations. Indeed, it can be described by the unitary representations of the group $SU(2)$, see [10]-paragraph 3.5.*

Remark 7 (On the interpretation of more general classical observables). *The functions listed in the left of the table imply products whose associated observables commute. This is true even for the components of the kinetic orbital moment, for instance $xp_y - yp_x$. Thereby, there is no problem to represent them as operators on the right of the table. But what choice could be done in the case of $xp_x = p_x x$. Should we take QP or PQ knowing that $QP \neq PQ$? There is an ambiguity concerning the order of these operations that will be discussed further in the text.*

Remark 8 (The expression **quantization** may have two distinct meanings that should be known and distinguished). *I. Todorov explains in his **lecture notes** how the word "quantization" may be used in the field of mathematical physics and the corresponding nuances:*

- The **geometric quantization** (called also **canonical**) is a mathematical approach to defining a quantum theory corresponding to a given classical theory. It is based on the symplectic geometry, and it is aimed to transit from classical mechanics to quantum mechanics. This is the passage from "symbols" to "operators";

- The **second quantization**. This second method furnishes a quantum description of multiple-particle systems (comprising a finite number of N particles, this is the **N -body problem**) with the help of the description (already quantic) of one particle. In fact, in order to take into account the spontaneous creation of particles, a quantum system must incorporate an infinite number of particles. The second quantization constructs a **functor** inside the category of Hilbert spaces, which sends \mathcal{H} towards the **Fock space** $\Gamma(\mathcal{H})$.

The passage from the classic world to the quantum framework can also be done at the level of the equations of motion. The Heisenberg equation (2.3) can be viewed as the extension of the **Liouville equation**. At all events, the condition (2.7) is a prerequisite. The issue is to determine what are the functional frameworks that allow to put it in concrete form.

Question 9. *What are (modulo isomorphisms) the set of triplets (\mathcal{H}, Q, P) involving two self-adjoint operators Q and P which act (as unbounded operators) on the complex Hilbert space \mathcal{H} and which are compatible with (2.7). And how to construct them?*

2.2. Translation into mathematics. The starting point is (2.7).

Lemma 10. *We assume (2.7). Then \mathcal{H} must be of finite dimension.*

This is a clear motivation to study vector spaces having infinite dimension!

Proof. As observed by **H. Weyl**, in the opposite case, taking the trace of (2.7), we obtain that $0 = -i\hbar \dim \mathcal{H}$ which is a contradiction. □

Lemma 11. *We assume (2.7). Then the operators Q and P are bounded.*

This is a motivation to study unbounded operators!

Proof. By contradiction again. By symmetry, we can suppose that Q is bounded. Since $P = P^*$, the action of $e^{\pm itP/\hbar}$ is unitary (this is the **Stone theorem** on the unitary semi-groups - to learn by heart). Besides:

$$(2.9) \quad e^{itP/\hbar} Q e^{-itP/\hbar} = Q + tId, \quad \forall t \in \mathbb{R}.$$

This is indeed true for $t = 0$. And, due to (2.7), the time derivative of the term on the left and on the right must coincide. The term on the left (2.9) is uniformly bounded in time. By contrast, the term on the right is not. This is the expected contradiction. □

It follows that the relation (2.7) can only be considered for unbounded operators acting on infinite dimensional spaces, with all the subtleties [4] that this implies! The first difficulty concerns already the test of the CCR. What can be said about PQ when the image of Q is not in the domain of P ?

A way to bypass these difficulties is to interpret (2.7) on the exponential side. One of the advantages is that $e^{\pm isQ/\hbar}$ and $e^{\pm itP/\hbar}$ become bounded operators on the whole space \mathcal{H} . By this way, we are lead to manipulate the auxiliary operators:

$$(2.10) \quad U_s := e^{isQ/\hbar} \in \mathcal{U}(\mathcal{H}), \quad V_t := e^{-itP/\hbar} \in \mathcal{U}(\mathcal{H})$$

which are amenable to the exponential version of the CCRs.

Definition 12. [Weyl commutation relations] This is the relation:

$$(2.11) \quad U_s V_t = e^{ist/\hbar} V_t U_s, \quad \forall (s, t) \in \mathbb{R}^2.$$

There is some heuristic argument allowing to deduce (2.11) from (2.9). Indeed, it suffices to expand U_s as a formal sum and then to use (2.9) in order to obtain:

$$\begin{aligned} V_t^{-1} U_s V_t &= \sum_{n=0}^{+\infty} \frac{1}{n!} V_t^{-1} \left(\frac{isQ}{\hbar} \right)^n V_t = \sum_{n=0}^{+\infty} \frac{1}{n!} \left(\frac{is}{\hbar} \right)^n V_t^{-1} Q^n V_t = \sum_{n=0}^{+\infty} \frac{1}{n!} \left(\frac{is}{\hbar} \right)^n (V_t^{-1} Q V_t)^n \\ &= \sum_{n=0}^{+\infty} \frac{1}{n!} \left(\frac{is}{\hbar} \right)^n (Q + tId)^n = e^{is(Q+tId)/\hbar} = e^{ist/\hbar} U_s. \end{aligned}$$

Remark 13. Be careful. The above argument is not correct. Indeed, for $n > 2$, the operator Q^n is not (always) well defined (because Q is an unbounded operator whose image is not necessarily contained in the domain of Q).

At this stage, the passage from (2.9) to (2.11) is not fully rigorous. To be convinced of that, we can provide with a counter-example. Take $\mathcal{H} = L_p^2([-1, 1])$ which is just L^2 with boundary periodic conditions. We work with $Q = x \times$ and $P = -i\hbar \partial_x$. We obtain that $U_s = e^{isx/\hbar} \times$. On the other hand (for all $n \in \mathbb{N}$), we have:

$$V_t e^{i\pi n x} = \sum_{j=0}^{+\infty} \frac{1}{j!} \left(\frac{-itP}{\hbar} \right)^j e^{i\pi n x} = \sum_{j=0}^{+\infty} \frac{1}{j!} (-i\pi n t)^j e^{i\pi n x} = e^{-i\pi n t} e^{i\pi n x} = e^{i\pi n(x-t)}.$$

The position $x - t$ is not sure to be in the interval $[-1, 1]$ but it falls inside this interval after an adequate translation. Let $m_{t,x}$ be the unique integer satisfying $-1 \leq x - t - 2m_{t,x} \leq 1$. Then:

$$e^{i\pi n(x-t)} = e^{i\pi n(x-t-2m_{t,x})}.$$

As the sequence of the $\psi_n(x) := e^{i\pi n x}$ with $n \in \mathbb{N}$ is dense in $L_p^2([-1, 1])$, we have

$$V_t \equiv S_{-t}, \quad (S_{-t}\psi)(x) := \psi(x - t - 2m_{t,x}).$$

Then we find that:

$$U_s V_t \psi_0 = U_s S_{-t} \psi_0 = U_s \psi_0 = e^{isx/\hbar}.$$

On the other hand:

$$e^{ist/\hbar} V_t U_s \psi_0 = e^{ist/\hbar} S_{-t} e^{isx/\hbar} = e^{ist/\hbar} e^{is(x-t-2m_{t,x})/\hbar} = e^{isx/\hbar} e^{-2ism_{t,x}/\hbar}.$$

We see here that in general $U_s V_t \neq e^{ist/\hbar} V_t U_s$.

Remark 14. Note however that, under reasonable assumptions, we can deduce (2.11) from (2.9). This is Nelson's theorem, see [8] - p. 15.

We will consider (2.11) as a substitute for (2.9). In the continuation of (2.11), we can define the unitary operator

$$\rho(t, s, r) := e^{ir/\hbar} V_t U_s \in \mathcal{U}(\mathcal{H}) := \{A \in \mathcal{L}(\mathcal{H}); A^{-1} = A^*\}.$$

By construction, we have:

$$(2.12) \quad \begin{aligned} \rho(t_1, s_1, r_1) \rho(t_2, s_2, r_2) &= (e^{ir_1/\hbar} V_{t_1} U_{s_1}) (e^{ir_2/\hbar} V_{t_2} U_{s_2}) \\ &= e^{i(r_1+r_2)/\hbar} V_{t_1} (U_{s_1} V_{t_2}) U_{s_2} \\ &= e^{i(r_1+r_2+s_1 t_2)/\hbar} V_{t_1+t_2} U_{s_1+s_2} \\ &= \rho(t_1 + t_2, s_1 + s_2, r_1 + r_2 + s_1 t_2). \end{aligned}$$

Remark 15. Let us introduce the group of matrices

$$(2.13) \quad \text{Heis}(\mathbb{R}) := \left\{ \begin{pmatrix} 1 & s & r \\ 0 & 1 & t \\ 0 & 0 & 1 \end{pmatrix}; (s, r, t) \in \mathbb{R}^3 \right\}.$$

The composition law of 3×3 unipotent matrices gives rise to:

$$\begin{pmatrix} 1 & s_1 & r_1 \\ 0 & 1 & t_1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & s_2 & r_2 \\ 0 & 1 & t_2 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & s_1 + s_2 & r_1 + r_2 + s_1 t_2 \\ 0 & 1 & t_1 + t_2 \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus, it furnishes composition rules which are similar to (2.12):

$$(s_1, r_1, t_1) \circ (s_2, r_2, t_2) = (s_1 + s_2, r_1 + r_2 + s_1 t_2, t_1 + t_2).$$

The set $\text{Heis}(\mathbb{R})$ equipped with the composition of matrices is called the *Heisenberg group* of order three that is associated with \mathbb{R} . We can also look at $\text{Heis}(\mathbb{R})$ as the *Lie algebra* \mathfrak{h}_1 whose exponential produces a Lie group (strictly speaking, the Heisenberg group). From the algebraic viewpoint, the use of the exponential, which is put in practice at the level of (2.10), is what allows to pass from the Lie algebra to the Lie group. The interesting reader can refer to the *lecture notes* of O. Schiffmann [9].

The choice of ρ made above does not give a symmetric role to s and t . We can prefer the following more symmetric version:

$$(2.14) \quad \varrho(t, s, r) := e^{i(r+st/2)/\hbar} V_t U_s$$

which furnishes

$$(2.15) \quad \varrho(0, 0, r) = e^{ir/\hbar} \text{Id}_{\mathcal{H}},$$

as well as

$$(2.16) \quad \begin{aligned} \varrho(t_1, s_1, r_1) \varrho(t_2, s_2, r_2) &= (e^{i(r_1+s_1 t_1/2)/\hbar} V_{t_1} U_{s_1}) (e^{i(r_2+s_2 t_2/2)/\hbar} V_{t_2} U_{s_2}) \\ &= e^{i(r_1+r_2+s_1 t_1/2+s_2 t_2/2)/\hbar} V_{t_1} (U_{s_1} V_{t_2}) U_{s_2} \\ &= e^{i(r_1+r_2+s_1 t_1/2+s_2 t_2/2+s_1 t_2)/\hbar} V_{t_1+t_2} U_{s_1+s_2} \\ &= e^{i[(r_1+r_2)+(s_1+s_2)(t_1+t_2)/2+(s_1 t_2-s_2 t_1)/2]/\hbar} V_{t_1+t_2} U_{s_1+s_2} \\ &= \varrho(t_1 + t_2, s_1 + s_2, r_1 + r_2 + (s_1 t_2 - s_2 t_1)/2). \end{aligned}$$

The variables s and t which are respectively associated with the position (Q) and the momentum (P), are dual of each other. The formula (2.16) highlights the *symplectic form*

$$\sigma((t_1, s_1), (t_2, s_2)) = (t_1, s_1) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} t_2 \\ s_2 \end{pmatrix} = (s_1 t_2 - s_2 t_1)$$

which incites to look at the vectors $v = (t, s) \in \mathbb{R}^2$ as being the elements of a two dimensional symplectic space.

Definition 16 (The Heisenberg algebra of a symplectic vector space). *Given a symplectic space (E, σ) , we can define the Lie algebra $\text{heis}(E, \sigma) = E \oplus \mathbb{R}e_0$ which is equipped with the Lie bracket*

$$[v_1 + r_1 e_0, v_2 + r_2 e_0] = \sigma(v_1, v_2) e_0.$$

Remark 17. The vectors $Q = (1, 0)$ and $P = (0, 1)$ form a symplectic basis of $E = \mathbb{R}^2$ whose representatives $\tilde{Q} = Q + 0 \times e_0$ and $\tilde{P} = P + 0 \times e_0$ in $\text{heis}(E, \sigma)$ satisfy:

$$[\tilde{P}, \tilde{P}] = 0, \quad [\tilde{Q}, \tilde{Q}] = 0, \quad [\tilde{P}, \tilde{Q}] = \sigma((0, 1), (1, 0)) e_0 = e_0.$$

By this way, the Heisenberg algebra allows to conceptualize (2.7), while making the link with the underlying symplectic structure.

Remark 18. We have

$$[[v_1 + r_1 e_0, v_2 + r_2 e_0], v_3 + r_3 e_0] = 0,$$

which shows that $\text{heis}(E, \sigma)$ is a nilpotent Lie algebra of rank two.

Definition 19 (Heisenberg group - Symplectic version). *The Heisenberg group of the symplectic space (E, σ) is the group $\mathcal{N} = E \oplus \mathbb{R}e_0$ equipped with the composition law*

$$(2.17) \quad (v_1 + r_1 e_0) \circ (v_2 + r_2 e_0) = v_1 + v_2 + (r_1 + r_2 + \sigma(v_1, v_2)/2)e_0, \quad (v_i, r_i) \in E \times \mathbb{R}.$$

In the particular case of the dimension two, when $E = \mathbb{R}^2$, we can identify $v + r e_0$ with the triplet (t, s, r) so that:

$$(v_1 + r_1 e_0) \circ (v_2 + r_2 e_0) = (t_1 + t_2, s_1 + s_2, r_1 + r_2 + \sigma(v_1, v_2)/2).$$

Definition 20 (Unitary representation). *A unitary representation of the group (\mathcal{N}, \circ) is a group morphism ϱ from \mathcal{N} to the set $\mathcal{U}(\mathcal{H})$ of unitary operators on \mathcal{H} . In other words $\varrho : \mathcal{N} \rightarrow \mathcal{U}(\mathcal{H})$ and we have:*

$$(2.18) \quad \varrho(v_1 + r_1 e_0) \varrho(v_2 + r_2 e_0) = \varrho((v_1 + r_1 e_0) \circ (v_2 + r_2 e_0)).$$

The representation is said to be non trivial when it is not constant (that is not equal to identity). It is irreducible when there is no subspace of \mathcal{H} different from $\{0\}$ or \mathcal{H} which is globally invariant by $\varrho(\mathcal{N})$.

For $E = \mathbb{R}^2$, with $\varrho(t_i, s_i, r_i) = \varrho(v_i + r_i e_0)$, we can recognize inside (2.16) the formula (2.18). Thereby, the question 9 extends into the following problem of classification.

Question 21. *What are the unitary representations of the Heisenberg group \mathcal{N} on the symmetric space (E, σ) which satisfy (2.15)?*

Remark 22. *The description (2.13) of $\text{Heis}(\mathbb{R})$ takes its values in the special linear group $SL(3)$. It is however not unitary. It does not comply with the specifications of question 21. We could also mention the existence of the theta representation.*

Before proceeding further, we can adopt a slightly different viewpoint. To this end, we need the following preliminary result (sometimes called Glauber formula) which must be seen as a particular case of the Baker-Campbell-Hausdorff formula.

Lemma 23. *[Glauber formula] Let $A \in \mathcal{L}(\mathcal{H})$ and $B \in \mathcal{L}(\mathcal{H})$ be two linear continuous operators which commute with their commutators. In other words*

$$(2.19) \quad [A, [A, B]] = [B, [A, B]] = 0.$$

Then:

$$(2.20) \quad e^A e^B = e^{A+B+[A,B]/2}.$$

Proof. If we remplace A by tA and B by tB with $t \in \mathbb{R}$ in (2.20), we recover a more general formula, which is

$$(2.21) \quad e^{tA} e^{tB} = e^{t(A+B)+t^2[A,B]/2}.$$

By exploiting (2.19), this can be interpreted into

$$h(t) = e^{t(A+B)}, \quad h(t) := e^{tA} e^{tB} e^{-t^2[A,B]/2}.$$

Compute

$$h'(t) = e^{tA} A e^{tB} e^{-t^2[A,B]/2} + e^{tA} e^{tB} B e^{-t^2[A,B]/2} - t e^{tA} e^{tB} e^{-t^2[A,B]/2} [A, B].$$

Using (2.19), we find that

$$\frac{d}{dt}(e^{-tB} A e^{tB}) = e^{-tB} [A, B] e^{tB} = [A, B],$$

which gives after integration

$$e^{-tB} A e^{tB} = A + t[A, B]$$

and then

$$e^{tA} A e^{tB} = e^{tA} e^{tB} e^{-tB} A e^{tB} = e^{tA} e^{tB} (A + t[A, B]).$$

We have therefore

$$h'(t) = h(t) (A + t[A, B] + B - t[A, B]) = h(t) (A + B),$$

and of course $h(0) = Id$. The function h satisfies the same ODE as $e^{t(A+B)}$ and it shares the same initial condition. The two expressions must coincide. □

Instead of working with U_s and V_t and then ϱ as in (2.14), we can prefer to exploit

$$\tilde{\rho}(t, s, r) := e^{i(tQ+sP+rId)/\hbar} \in \mathcal{U}(\mathcal{H}).$$

As

$$[t_2Q + s_2P + r_2Id, t_1Q + s_1P + r_1Id] = t_2s_1[Q, P] + s_2t_1[P, Q] = i\hbar(s_1t_2 - s_2t_1),$$

Glauber's formula gives directly access to the laws of the Heisenberg group, namely

$$\tilde{\rho}(t_2, s_2, r_2) \tilde{\rho}(t_1, s_1, r_1) = \tilde{\rho}(t_1 + t_2, s_1 + s_2, r_1 + r_2 + (s_1t_2 - s_2t_1)/2).$$

We can also interpret the preceding manipulations in the perspective of complex analysis. Given $z = s + it$ and $z' = s' + it'$, define

$$W_z := e^{-i(sP-tQ)}, \quad W_{z'} := e^{-i(s'P-t'Q)}.$$

With $A = -i(sP - tQ)$ and $B = -i(s'P - t'Q)$, we obtain that

$$[A, B] = -[sP - tQ, s'P - t'Q] = st'[P, Q] + ts'[Q, P] = i\hbar(ts' - st') Id$$

which obviously commutes with A and B . Although the operators $sP - tQ$ and $s'P - t'Q$ are not bounded, we will (as it was the case at the level of Definition 12) ignore the complications related to the domains of the operators. We apply Lemma 23. By this way, we find that

$$(2.22) \quad W_z W_{z'} = e^{i\hbar(ts' - st')/2} W_{z+z'} = e^{-i\hbar \text{Im}(z\bar{z}')/2} W_{z+z'} = e^{-i\hbar \text{Im}\langle z, z' \rangle/2} W_{z+z'}.$$

This is another version of Weyl commutation relations in which W appears as a projective representation of the group $(\mathbb{C}, +)$. According to the context, it may be preferable to deal with the real and symplectic facets through (12) or to opt for the complex formulation (2.22).

3. THE WAVE MECHANICS

This is about a line of research initiated by E. Schrödinger from 1926. But we have first to mention the pioneering works of L. De Broglie (undertaken in 1924 in his thesis on the wave structure of electrons). L. De Broglie is a french mathematician and physicist who adopted the opposite direction which goes from waves to particles, that is:

Any moving particle or object of mass m and velocity v has an associated wave.

A wave may be represented by a function $\psi(t, x)$ defined on the spacetime. If we suppose that it is sufficiently localized and integrable, it can be interpreted at the time t as belonging to $L^2(\mathbb{R}^d)$, with $d = 1$ or 2 or 3 according to the dimension of the studied phenomenon. A vision of the type "discret object" can always be applied by selecting an orthonormal basis $e_1, e_2, \dots, e_n, \dots$ of the space $L^2(\mathbb{R}^d)$, often denoted by $|e_1\rangle, |e_2\rangle, \dots, |e_n\rangle, \dots$ by physicists. This basis has a dual basis $\langle e_1|, \langle e_2|, \dots, \langle e_n|, \dots$ which is characterized by

$$\langle e_i | e_j \rangle \equiv (e_i, e_j) = \int_{\mathbb{R}^d} \bar{e}_i(x) e_j(x) dx = \delta_{ij}, \quad \forall (i, j) \in \mathbb{N}^2.$$

Any element $\psi(t, \cdot)$ of $L^2(\mathbb{R}^d)$ can be decomposed into

$$\psi(t, \cdot) = \sum_{n=1}^{+\infty} c_n(t) |e_n\rangle, \quad c_n(t) := \langle e_n | \psi(t, \cdot) \rangle.$$

By this way, we can identify *states* $\psi(t, \cdot) \in \mathcal{H} \equiv L^2(\mathbb{R}^d)$ with vectors $(c_n(t))_n \in \ell^2(\mathbb{N}; \mathbb{C}) \subset \mathbb{C}^{\mathbb{N}}$. The viewpoint of Schrödinger is to fix the observables, and to see the states as waves $\psi(t, \cdot)$ in $L^2(\mathbb{R}^d; \mathbb{C})$ evolving according to:

$$(3.1) \quad i \hbar \partial_t \psi = H \psi, \quad H : \text{Dom}(H) \subset L^2 \rightarrow L^2.$$

To simplify, we will suppose that the operator H does not depend on the time t . Then, for an electron of the atom which is subjected to some electromagnetic potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$ created by the protons of the nucleus, in a first approximation, we can take:

$$(3.2) \quad H = -\frac{\hbar^2}{2m} \Delta_x + V(x), \quad \Delta_x = \sum_{j=1}^d \partial_{x_j}^2, \quad V \in C^\infty(\mathbb{R}^d; \mathbb{R}).$$

We see here that the action of H is typically achieved through some self-adjoint unbounded operator [4]. The choice of H comes often from a lagrangian or hamiltonian formulation of the equations. The observable H corresponds to the computation of an energy. The state of the system evolves according to:

$$\psi(t) = W(t)\psi(0), \quad W(t) := e^{-itH/\hbar}.$$

This means that the operator H plays the role (in the sense of [Stone's theorem](#) [4]) of a *generator* of time translations of the wave functions. Knowing H , a well adapted choice (from the viewpoint of physical interpretations) consists in selecting (when it exists, see the course on spectral theory) the basis made of eigenvectors $|e_1\rangle, |e_2\rangle, \dots, |e_n\rangle, \dots$ (associated to the eigenvalues E_n) generated by H . Then, we have:

$$W(t)\psi(0) = \sum_{n=1}^{+\infty} e^{-itE_n/\hbar} c_n(0) |e_n\rangle.$$

Remark 24 (The case of free particles). *When $V \equiv 0$, we can solve the equation (3.1) whose coefficients are then constant by a Fourier transform. This yields:*

$$W(t)\psi(0) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \varphi_\hbar(p) e^{-ip^2 t/(2m\hbar)} e^{ixp/\hbar} dp,$$

where $\varphi_\hbar(p)$ is obtained from $\psi(0)$ by Fourier transform (with parameter \hbar).

The propagator $W(t)$ is a unitary operator. Hence, the L^2 -norm of $\psi(t, \cdot)$ is equal to 1 if the L^2 -norm of the initial data $\psi(0)$ has been normalized. Thereupon, the square $|\psi(t, x)|^2$ can be interpreted (as first suggested by N. Bohr) as a probability density of the presence of the particle at (t, x) . The mean value $\langle A \rangle(t)$ of the *observable* A against $\psi(t)$ is:

$$\langle A \rangle(t) := \langle \psi(t), A\psi(t) \rangle = \langle \psi(0), A(t)\psi(0) \rangle, \quad A(t) := W(t)^* A W(t).$$

In the approach of Heisenberg, it is the state $\psi(0)$ which is fixed whereas the operator A moves with time as $A(t)$. From the definition of $A(t)$, we can easily recover the equation of Heisenberg. Indeed, knowing that

$$[W(t), H] = 0, \quad W(t)^* W(t) = W(t) W(t)^* = \text{Id},$$

we can obtain as expected that:

$$\begin{aligned} i \hbar \partial_t A(t) &= -W(t)^* H A W(t) + W(t)^* A H W(t) \\ &= -W(t)^* H W(t) W(t)^* A W(t) + W(t)^* A W(t) W(t)^* H W(t) = [A(t); H]. \end{aligned}$$

Remark 25 (The Ehrenfest's theorem). Compute

$$\frac{d}{dt}\langle A \rangle(t) = \frac{1}{i\hbar} \langle \psi(0), [A(t); H]\psi(0) \rangle = \frac{1}{i\hbar} \langle [A(t); H] \rangle.$$

In the case of an hamiltonian of the type $H(Q, P) = V(Q) + (P^2/2m)$, this leads to:

$$\begin{cases} \frac{d}{dt}\langle Q \rangle(t) = \frac{1}{i\hbar} \langle [Q; P^2/2m] \rangle \\ \frac{d}{dt}\langle P \rangle(t) = \frac{1}{i\hbar} \langle [P; V(Q)] \rangle. \end{cases}$$

The relation (2.7) furnishes directly:

$$[Q; P^2/2m] = i\hbar P/m.$$

For an analytical potential $V(\cdot)$, this gives access to:

$$[P; V(Q)] = \sum_{n=0}^{+\infty} V_n [P; Q^n] = -i\hbar \sum_{n=1}^{+\infty} nV_n Q^{n-1} = -i\hbar V'(Q).$$

Thus, we have to deal with:

$$\begin{cases} \frac{d}{dt}\langle Q \rangle(t) = \langle P \rangle/m, \\ \frac{d}{dt}\langle P \rangle(t) = -\langle V'(Q) \rangle. \end{cases}$$

Assuming that $\langle V'(Q) \rangle$ can above be replaced by $V'(\langle Q \rangle)$, we find the *Hamilton-Jacobi equations* of a classical particle located at $(\langle Q \rangle, \langle P \rangle)$ and subject to the hamiltonian:

$$H(\langle Q \rangle, \langle P \rangle) = V(\langle Q \rangle) + (\langle P \rangle^2/2m).$$

This argument furnishes a correspondence (through the computation of mean values) between the quantum and classical situations. However, in general, the mean value of $V'(Q)$ does not coincide with V' evaluated at $\langle Q \rangle$. It follows that significant differences may occur between the quantum and classical dynamics (the *quantum tunnelling* [6] is one of them).

Remark 26 (The perspective of microlocal analysis). It is possible to look at the action of the operator $A(t) : \mathcal{S}(\mathbb{R}^d) \rightarrow \mathcal{S}'(\mathbb{R}^d)$ through its symbol $\sigma(t, x, \xi)$. Indeed, the action of $A(t)$ may be viewed as the one of an element $\sigma(t, \cdot) \in \mathcal{S}'(\mathbb{R}^d \times \mathbb{R}^d)$, and we can read the time evolution of the distribution $\sigma(t, \cdot)$ as a dynamic in the phase space. Another method, often more illustrative but less general, consists in studying the action of $A(t)$ on a specific state. This amounts to consider the *Husimi representation* (see [6] - paragraph 1.3.2.2) of a quantum state $\psi(t, \cdot)$ which is a special solution to the Schrödinger equation. An alternative method is to exploit the *Segal-Bargmann transform*.

Remark 27 (Come back to atomic spectroscopy). The values obtained for the E_n depend of course on the choice of H . For a coulombian potential (of the type $1/|x|$ and not $|x|^2$ as for the harmonic oscillator), we recover the $1/n^2$ of Rydberg's formula with for each $E_n = 1/n^2$ a multiplicity $(2k+1)n^2$ (where k is the spin - this is $1/2$ for the electron). In practice, we can observe near each E_n the existence of gaps among which:

- the *fine structure* which describes the duplication of the spectral line associated with E_n . This effect is of relativistic origin. It can be explained by resorting to the Dirac equations (the hamiltonian becomes with values in \mathbb{C}^4), see [10]-paragraph 4.3;

- the *Lamb shift* which is due to the interactions between the fluctuations of the vacuum and the hydrogen electron on its orbitals. It is necessary to use the second quantization to explain this phenomenon;

- the *hyperfine structures* which are issued from the interactions between the magnetic dipoles induced by the nuclei and the electrons.

The theoretical description of these different aspects can be made by some modeling and then by the spectral theory of adequate operators.

4. THE STONE VON-NEUMANN THEOREM

Let us come back to the question 9. At this stage, we have focussed on two conceptions which are apparently distinct: the matrix and wave approaches. There is however some analogy between the two, which is related to (2.7). Indeed, consider the (unbounded) position operator \tilde{Q}_j and momentum operator \tilde{P}_j acting according to:

$$\tilde{Q}_j \psi = x_j \psi, \quad \tilde{P}_j \psi = -i\hbar \partial_{x_j} \psi.$$

For the sake of simplicity, we can work in space dimension one (with $d = 1$ and $x \in \mathbb{R}$). The involved operators are then just:

$$\tilde{Q} = x \times, \quad \tilde{P} = -i\hbar \partial_x.$$

As already explained, the first step in the quantization of a particle is to replace the position x and the momentum p by the operators \tilde{Q} and \tilde{P} . Obviously:

$$[\tilde{P}, \tilde{Q}] \psi = -i\hbar \partial_x(x\psi) + ix\hbar \partial_x \psi = -i\hbar \psi.$$

The two operators \tilde{Q} and \tilde{P} are therefore compatible with (2.7). Besides, a formal calculus (which for ψ in the Schwartz space does not raise problems about domains and which can be justified by the differential characterization in Stone's theorem) furnishes

$$\begin{aligned} \tilde{U}_s \psi &:= e^{is\tilde{Q}/\hbar} \psi = \sum \frac{1}{n!} (is\tilde{Q}/\hbar)^n \psi = \sum \frac{1}{n!} (isx/\hbar)^n \psi = e^{isx/\hbar} \psi, \\ \tilde{V}_t \psi &:= e^{-it\tilde{P}/\hbar} \psi = \sum \frac{1}{n!} (-it\tilde{P}/\hbar)^n \psi = \sum \frac{1}{n!} (-t)^n \partial_x^n \psi = \psi(x-t). \end{aligned}$$

As expected, the actions of \tilde{U}_s and \tilde{V}_t make sense on the whole space $L^2(\mathbb{R}^d)$. We also see that the position operator \tilde{Q} and the momentum operator \tilde{P} are the generators of translation groups respectively in momentum p and in position x (see [6]-paragraph 2.1). A novelty is that explicit formulas are available. They allow to test directly (without passing through \tilde{Q} and \tilde{P}) the validity of (2.11). Indeed, we have:

$$(4.1) \quad \tilde{U}_s \tilde{V}_t \psi = e^{isx/\hbar} \psi(x-t) = e^{ist/\hbar} e^{is(x-t)/\hbar} \psi(x-t) = e^{ist/\hbar} \tilde{V}_t \tilde{U}_s \psi.$$

Knowing (4.1) and applying (2.14), we can effectively construct a unitary representation of the group (\mathcal{N}, \circ) which is built on $L^2(\mathbb{R})$. This is the (one dimensional version of the) Schrödinger representation. There are other explicit representations. For instance, V. Bargmann who was the assistant of A. Einstein at the Institute for Advanced Study in Princeton (from 1937 to 1946) has introduced (in 1961) another representation which is based on the *Segal-Bargmann space*.

Theorem 28. [Stone Von-Neumann theorem] *A non trivial unitary irreducible representation $\varrho : \mathcal{N} \rightarrow \mathcal{U}(\mathcal{H})$ which is such that $\varrho(re_0) = e^{ir/\hbar} Id_{\mathcal{H}}$ is necessarily unitary equivalent to the Schrödinger representation.*

The proof is detailed for instance in [7]-paragraph 3.4.

The formula (2.18) and the condition $\varrho(re_0) = e^{ir/\hbar} Id_{\mathcal{H}}$ have been introduced from (2.11) and from (2.15). We will be satisfied below with working on representations deduced from Q and P through the passage to the exponential as in (2.10). In this context, the notion of irreducibility is translated into the following condition.

Definition 29. *Operators Q and P satisfying (2.11) act in an irreducible way on \mathcal{H} if the only closed subspaces of \mathcal{H} which are invariant under the action of U_s and V_t are $\{0\}$ and \mathcal{H} .*

Starting from (2.11), we can now formulate the following alternative to Theorem 28.

Theorem 30. *[Simplified version in dimension $d = 1$ of the Stone Von-Neumann theorem] Let Q and P be two self-adjoint operators acting in an irreducible way on \mathcal{H} and satisfying the Weyl commutation relations (2.11). There exists a unitary transformation $\mathfrak{U} : \mathcal{H} \rightarrow L^2(\mathbb{R})$ such that:*

$$\mathfrak{U} e^{isQ/\hbar} \mathfrak{U}^{-1} = e^{is\tilde{Q}/\hbar}, \quad \mathfrak{U} e^{-itP/\hbar} \mathfrak{U}^{-1} = e^{-it\tilde{P}/\hbar}.$$

According to this statement, the representations obtained by Heisenberg and Schrödinger are unitary equivalent. In other words, they are two facets of a same object. Or working with $\mathcal{H} = L^2(\mathbb{R})$ and (3.1) allows to put (2.7) in a concrete form (without losing information).

Remark 31. *As already explained, the relations (2.11) are built through a unitary representation of (\mathcal{N}, o) for which $\mathcal{N} = E \oplus \mathbb{R}e_0$ where E is of finite dimension (namely even). There exist more general situations for which E is of infinite dimension. This is typically the case in quantum field theory. Then, there is an infinite number of degrees of freedom, often indexed by the wave vectors $k \in \mathbb{R}^3$. We lose the uniqueness of the unitary transformation (except if we impose supplementary restrictions [9]) but we keep the existence of a reduction to the Schrödinger equation.*

Our aim is to prove Theorem 30. This is the occasion to talk about the harmonic oscillator (lesson 2), about the [uncertainty principle](#) (lesson 3) and about various problems of quantization (lesson 4).

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