M2 course notes
Microlocal analysis
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# Sessions about quantum mechanics 

Chapter 2 on

## The quantum harmonic oscillator (physical motivations and analysis)

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## 0. Introduction

We start by explaining the objectives and the motivations. Then, we describe at length the historical context.
0.1. Purpose. Be aware of the quantum harmonic oscillator in its algebraic facets (manipulation of eigenvalues issued from operators satisfying canonical commutation relations) and analytic aspects (study of eigenfunctions obtained by looking at the Schrödinger representation).
0.2. Motivations. A dynamical system moving in a potential near a stable equilibrium position, that is near a minimum of the potential, can be modeled by the harmonic oscillator, at least for small oscillations. The picture below shows:

- the comparison for a diatomic molecule between the (blue) curve corresponding to the "real" potential (represented by the Morse potential) and the (green) curve for the harmonic oscillator;
- the differences between the (quantum) energy levels that are associated to both cases.


The quantum harmonic oscillator appears in condensed matter physics in order to describe the vibrations of a crystal structure in the form of solide cristallin sous la forme de phonons. Above all, it is a basic model to understand how the quanta of energy operate during radiation. We can refer to the photons of electromagnetism but also to the whole set of elementary particles in the standard model.
0.3. Historical context. The harmonic oscillator was first used for the description of different types of pendulums (paragraph 0.4). Its quantum version was exploited to explain the emission spectrum of atoms. Then, it has played an essential role in the quantum formulation of the interactions between radiations and matter, in quantum electrodynamics (paragraph 1.1) and then in quantum field theory.
0.4. The spring-mass system. In classical mechanics, a particle of position $q \in \mathbb{R}^{d}$ and mass $m$ moves in Galilean reference frame according to the fundamental principle of dynamics (the well-known Newton's laws of motion):

The change of motion of an object is proportional to the force $\vec{F}$ impressed and it is made in the direction of the straight line in which the force is impressed

$$
(p=m \dot{q}=\vec{F})
$$

In the case of a conservative force coming from a potential $V(q)$, we obtain the canonical equations of Hamilton:

$$
\left\{\begin{array}{l}
\dot{q}=p / m=\nabla_{p} H  \tag{0.1}\\
\dot{p}=-\nabla_{q} V(q)=-\nabla_{q} H
\end{array}\right.
$$

which imply the hamiltonian

$$
H(q, p):=\underset{2}{V}(q)+\frac{|p|^{2}}{2 m}
$$

Near the equilibrium position (say placed at the origin $q=0$ ) in which $\nabla_{q} V(0)=0$, we can approximate the potential function by its Taylor expansion:

$$
V(q)=V(0)+\frac{1}{2}^{t} q D_{q}^{2} V(0) q+o\left(|q|^{2}\right)
$$

Near a non degenerate minimum, the quadratic form associated with $D_{q}^{2} V(0)$ is positive definite. At first approximation, we can replace $V(q)$ by its Taylor expansion (up to the order two). In particular for the horizontal spring-mass system without damping $(d=1)$, we ecover $V(q)=$ $k q^{2} / 2$ where $k$ is the spring's stiffness.


For such a choice, the solutions of (0.1) satisfy:

$$
\begin{equation*}
\ddot{q}+\omega_{0}^{2} q=0, \quad \omega_{0}:=\sqrt{k / m} \tag{0.2}
\end{equation*}
$$

The solutions which are issued (with zero speed) from the position $q_{0}$ at the time $t=0$ have the form $q(t)=q_{0} \cos (\sqrt{m k} t)$. The trajectories drawn in position (after projection according to $q$ ) or in the phase space (in both $p$ and $q$ ) look like respectively as in the pictures on the left (oscillations) or on the right (concentric circles in the phase portrait):


To conclude this introduction, it is worth emphasizing that the previsions provided by the quantum harmonic oscillator are in accordance with experimental phenomena among which we can mention:

- the Lamb shift which was not forecast by Dirac and which was first computed by H. Bethe. It is due to the interaction between the quantum fluctuations of the vacuum and the electron;
- the Casimir effect, see [4]-paragraph 2.2.4.

This theory is at the root of a promising research field, quantum optics, which has been rewarded in recent years by Nobel Prizes in Physics for S. Haroche, D. Wineland, R. J. Glauber, C. CohenTannoudji and also recently A. Aspect (2022).

## 1. The quantum harmonic oscillator

We start with preliminary considerations.
1.1. Towards a quantum model. The case of a stable minimum is quite common in quantum mechanics because, at low temperatures, the particles tend to go near their equilibrium position, which is the position having the lower energy. As already explained, the (first) quantization of the classical hamiltonian replaces the variables $q$ and $p$ by the position operator $Q=q \times$ and the impulsion operator $P=-i \hbar \partial_{q}$ which satisfy the canonical commutation relation $[P, Q]=-i \hbar I d$. By this way, we find the hamiltonian operator:

$$
\begin{equation*}
H:=\left(Q^{2}+P^{2}\right) / 2 . \tag{1.1}
\end{equation*}
$$

From there, the equation which comes to replace ( 0.2 ) is the Schrödinger equation:

$$
\begin{equation*}
2 i \hbar \partial_{t} \psi=\hbar\left(-\partial_{q}^{2}+q^{2}\right) \psi . \tag{1.2}
\end{equation*}
$$

The model (1.2) which has been obtained by analogy with (0.2) is called the quantum harmonic oscillator. It describes the time evolution of an isolated quantum particle. For the sake of simplicity, we will work in space dimension 1 and with the normalized version (that is with $\hbar=1$ ). But keep in mind that the scales are essential to perform ultimately physical interpretations.
Remark 1 (Return to Ehrenfest's theorem). We can associate with (1.2) initial data chosen in the form of Gaussian wave packets:

$$
\psi(0, x)=\psi_{0}(x):=\frac{1}{\left(\pi \sigma^{2}\right)^{1 / 4}} \exp \left(i \frac{p_{0} x}{\hbar}\right) \exp \left(-\frac{\left(x-x_{0}\right)^{2}}{2 \sigma^{2}}\right), \quad\left(x_{0}, p_{0}, \sigma\right) \in \mathbb{R}^{2} \times \mathbb{R}_{+}^{*}
$$

The mean values $\langle Q\rangle(0)$ and $\langle P\rangle(0)$ of the observables $Q$ and $P$ tested again the state $\psi_{0}$ are:

$$
\langle Q\rangle(0)=\left\langle\psi_{0}, Q \psi_{0}\right\rangle=\int_{\mathbb{R}} x\left|\psi_{0}(x)\right|^{2} d x=x_{0}, \quad\langle P\rangle(0)=\left\langle\psi_{0}, P \psi_{0}\right\rangle=i \hbar \int_{\mathbb{R}} p \bar{\psi}_{0}(x) \psi_{0}^{\prime}(x) d x=p_{0} .
$$

We can prove, for instance by computing the kernel of the propagator, that the solution of (1.2) stays at all times $t \in \mathbb{R}_{+}^{*}$ a gaussian (with parameters $x_{t}, p_{t}$ and $\sigma$ ). To determine it, it suffices to give access to

$$
x_{t}:=\langle Q\rangle(t), \quad p_{t}:=\langle P\rangle(t) .
$$

A very practical way to achieve this is Ehrenfest's theorem. Indeed, in the case of a the quadratic energy (1.1), we find that $\left\langle V^{\prime}(Q)\right\rangle=\langle Q\rangle$ so that:

$$
\left\{\begin{array}{l}
\dot{x}_{t}=p_{t} / m \\
\dot{p}_{t}=-q_{t}
\end{array}\right.
$$

The motion of the mean values is then the one of a classical particle around which the gaussian states propagate without deformation (see [3] for simulations).
The focus on (1.2) dates back to the works of the britanish physicist P. Dirac who, in the 1920s, was the first to establish the rate of spontaneous emission. The use of equation (1.2) allows to conceptualize the interaction between radiation and matter. In particular, P. Dirac will describe the electromagnetic field (see [4]-paragraph 2.2.4 for further precisions) by the help of a set of discrete harmonic oscillators (indexed by wave vectors) and by associating to the particles the ladder operators:

$$
\begin{array}{ll}
a:=(Q+i P) / \sqrt{2}, & \\
c:=a^{*}=(Q-i P) / \sqrt{2}, & \\
\text { raisising operator. }
\end{array}
$$

These operators lead to a decomposition of $H$ as indicated below.
Lemma 2. The operator $H$ can be written as $H=N+(I d / 2)$ where $N:=c a=a^{*} a$ is called the particle number operator.

Proof. By definition:

$$
H=\frac{1}{2}(Q-i P)(Q+i P)-\frac{i}{2}[Q, P]=a^{*} a-\frac{i}{2} \times i I d=N+(I d / 2) .
$$

The operator $H$ appears as a symmetric operator satisfying (for all function $\psi$ of class $C^{\infty}$ with compact support):

$$
\begin{equation*}
\langle\psi, H \psi\rangle=\|a \psi\|^{2}+\frac{1}{2}\|\psi\|^{2} \geq \frac{1}{2}\|\psi\|^{2} \tag{1.3}
\end{equation*}
$$

This is an unbounded operator on $\mathcal{H}=L^{2}(\mathbb{R})$. It becomes self-adjoint on a suitable domain. We can refer to [1]-paragraphs 2.6 .3 and 6.2 .1 as well as to [5]-paragraph 12 for all possible characterizations of the domain of $H$. The following choice is appropriate:

$$
\operatorname{Dom} H=\left\{\psi \in L^{2}(\mathbb{R}) ; \partial_{q} \psi \in L^{2}(\mathbb{R}), \partial_{q q}^{2} \psi \in L^{2}(\mathbb{R}), q^{2} \psi \in L^{2}(\mathbb{R})\right\}
$$

Since $H$ is self-adjoint, its spectrum $\sigma(H)$ is real [1,7]. The same applies to its ponctual spectrum $\sigma_{p}(H)$. Moreover, from the lower bound (1.4), we can assert that:

$$
\begin{equation*}
\sigma_{p}(H) \subset \sigma(H) \subset[1 / 2,+\infty[ \tag{1.4}
\end{equation*}
$$

The elements $\lambda$ of $\sigma_{p}(H)$ can be interpreted as quanta of energy. Indeed, the third postulate of quantum mechanics asserts that these are the only mesurable energies. Hence the need of identifying all eigenvalues $\lambda$ of the operator $H$ as well as all eigenfunctions $\psi_{\lambda}$ of $H$. We denote by $E_{\lambda}$ the eigenspace of $H$ associated with $\lambda$. It should be borne in mind that the equation (1.2) has special solutions given by:

$$
\begin{equation*}
\psi(t)=e^{-i \lambda t} \psi_{\lambda}, \quad \forall \psi_{\lambda} \in E_{\lambda}:=\{\psi \in \operatorname{Dom} H ;(H-\lambda I d) \psi=0\} \tag{1.5}
\end{equation*}
$$

Remark 3 (Stationnary states). Physically, the wave functions $\psi$ and $\mu \psi$ for $\mu \in \mathbb{C}^{*}$ represent the same physical state. What matters is the probability density induced by the function $\psi$, the one which is obtained by normalizing $\psi$ in $L^{2}(\mathbb{R})$. The vector $\psi$ must therefore be interpreted as an element of the projective Hilbert space $P(\mathcal{H})$. Seen in this light, the rotation of $\psi_{\lambda}$ observed when the time evolves at the level of (1.5) has no physical effect. This is why it is sometimes said that the solutions described by (1.5) are stationary states.
Besides, along this line, we can observe that, for the quantum states $\psi$ obtained at the level of (1.5), the mean value of the observable $A \in \mathcal{L}(\mathcal{H})$ does not change since

$$
\langle\psi(t)| A|\psi(t)\rangle=\left\langle e^{-i \lambda t} \psi_{\lambda}\right| A\left|e^{-i \lambda t} \psi_{\lambda}\right\rangle=\left\langle\psi_{\lambda}\right| A\left|\psi_{\lambda}\right\rangle
$$

First and foremost, let us begin by checking that the lower bound $1 / 2$, which may be achievable in view of $(1.4)$, is indeed in $\sigma_{p}(H)$. To this end, we try to identify the set of corresponding eigenvectors $\psi_{0}$. In view of Lemma 2, this amounts to solve

$$
\left(-\partial_{q}+q\right)\left(\partial_{q}+q\right) \psi_{0}=0, \quad \psi \in \operatorname{Dom} H
$$

which implies that

$$
\left\langle\psi_{0},\left(-\partial_{q}+q\right)\left(\partial_{q}+q\right) \psi_{0}\right\rangle=\left\langle\left(\partial_{q}+q\right) \psi_{0},\left(\partial_{q}+q\right) \psi_{0}\right\rangle=\left\|\left(\partial_{q}+q\right) \psi_{0}\right\|_{L^{2}(\mathbb{R})}^{2}=0
$$

or equivalently that

$$
\begin{equation*}
\left(\partial_{q}+q\right) \psi_{0}=0 \tag{1.6}
\end{equation*}
$$

The functions $\psi_{0}(q)=C e^{-q^{2} / 2}$ with $C \in \mathbb{C}$ are (by Cauchy-Lipschitz theorem) the only solutions of (1.6). And they are in Dom $H$. Thus, they can be selected.
(1.7) The eigenspace $E_{1 / 2}$ that is associated with the eigenvalue $1 / 2$ is of dimension one.

The eigenspace $E_{1 / 2}$ is spanned by a gaussian which is called the ground state because it corresponds to the state having the minimal energy. In quantum physics, the vacuum energy is never zero (it is $1 / 2$ in dimensionless units)!

Remark 4. The classical situation is quite different. Indeed, a spring placed in the equilibrium position with a zero speed inherits a total energy which is equal to zero. The above phenomenon is remarkable. It is at the origin of the quantum fluctuation which manifests itself as the spontaneous creation of a pair of virtual particles made of a particle and its corresponding antiparticle. The
reader can find in [2]-paragraph 5.1.2 some interesting comparison between the classical and quantum configurations.

The purpose of the rest of this section is to show that the use of the functions $\psi_{\lambda}$ gives access to a complete spectral decomposition of $H$. In this perspective, the theorem of Stone Von Neumann is instructive because it claims that we can achieve the spectral study of $H$, knowing that the Heisenberg and Schrödinger approaches are equivalent. Thus, the information provided by the algebraic (Paragraph 1.2) and analytical (Paragraph 1.3) methods complement each other to furnish a global vision. Now, some difficulties are easier or faster to deal with on one side than the other. The algebraic approach presented in Subsection 1.2 below is not sufficient to close the subject. We also need the analytical viewpoint. We will underline the arguments which become simpler with the analytical perspective by the mention An $\star$ with $\star \in \mathbb{N}^{*}$.
1.2. The algebraic approach. The matter is to initiate the spectral discussion by looking at the position operator $Q=q \times$ and at the impulsion operator $P=-i \partial_{q}$ only through the algebraic relations:

$$
\begin{equation*}
P=P^{*}, \quad Q=Q^{*}, \quad H=\left(Q^{2}+P^{2}\right) / 2, \quad[P, Q]=-i I d \tag{1.8}
\end{equation*}
$$

We do not specify the Hilbert spaces $\mathcal{H}$ on which acts $H$, and we skip (for the moment) questions related to the choice of domains (which are however pointed by An*).
An1: We complete (1.8) by adding the preliminary condition (1.7), namely:

$$
\begin{equation*}
\operatorname{dim} E_{1 / 2}=\operatorname{dim} \operatorname{ker}(H-1 / 2)=1 \tag{1.9}
\end{equation*}
$$

According to Lemma 2, it is equivalent to study $H$ (modulo the soustraction of $1 / 2$ ) or the properties of the particle number operator $N$. The condition (1.9) is the same as dim ker $N=1$. The eigenspace of $N$ is generated by a vector $\psi_{0} \neq 0$ (with $\psi_{0}$ in the domain of $H$ ). Since

$$
0=\left\langle\psi_{0} \mid N \psi_{0}\right\rangle=\left\langle a \psi_{0} \mid a \psi_{0}\right\rangle=\left\|a \psi_{0}\right\|^{2}
$$

this vector $\psi_{0}$ is also in the kernel of $a$. Because $\operatorname{ker} a \subset \operatorname{ker} N$, the kernel of $a$ is of dimension one, and it is spanned by $\psi_{0}$.

Lemma 5 (The canonical commutation relation interpreted in terms of $c$ and $a$ ). We find that $[a, c]=I d$. More generally, for all $n \in \mathbb{N}^{*}$, we have:

$$
\begin{equation*}
\left[a, c^{n}\right]=n c^{n-1} . \tag{1.10}
\end{equation*}
$$

Proof. Elementary computations furnish

$$
[a, c]=\frac{1}{2}[Q+i P, Q-i P]=\frac{i}{2}[P, Q]-\frac{i}{2}[Q, P]=I d .
$$

Suppose that (1.10) is verified for $n$. Then

$$
\left[a, c^{n+1}\right]=\left[a, c^{n}\right] c+c^{n}[a, c]=n c^{n-1} c+c^{n} c=(n+1) c^{n},
$$

which shows the result by induction.

Lemma 6. The vectors $\psi_{n}:=c^{n} \psi_{0}$ with $n \in \mathbb{N}$, sometimes just denoted by $|n\rangle$, are eigenvectors of $N$ associated with the eigenvalues $n$. They are mutually orthogonal.
An2: Nothing guarantees that the $\psi_{n}$ - and in particulier $\psi_{0}$ - are in the domain of $N$. This hypothesis, which is here implicitly viewed as being satisfied, can be verified by analysis.
Proof. By definition of $\psi_{0}$, this is true for $n=0$. We statrt by proving the relations:

$$
\begin{equation*}
[N, a]=[c, a] a=-a, \quad[N, c]=-c[c, a]=c . \tag{1.11}
\end{equation*}
$$

Then, we proceed by induction. Knowing that $N \psi_{n}=n \psi_{n}$, we can recover that

$$
N \psi_{n+1}=[N, c] \psi_{n}+c N \psi_{n}=c \psi_{n}+n c \psi_{n}=(n+1) \psi_{n+1}
$$

and so on. Besides, for $n \neq m$, we have

$$
\left\langle\psi_{n}, N \psi_{m}\right\rangle=m\left\langle\psi_{n}, \psi_{m}\right\rangle=\left\langle N^{*} \psi_{n}, \psi_{m}\right\rangle=\left\langle N \psi_{n}, \psi_{m}\right\rangle=n\left\langle\psi_{n}, \psi_{m}\right\rangle .
$$

For $m \neq n$, this is possible only if $\left\langle\psi_{n}, \psi_{m}\right\rangle=0$.

The operator $c$ is qualified as raising because it allows to reveals from the fundamental state $\psi_{0}$ the $n^{\text {th }}$ quantum level of energy by successive jumps.
Lemma 7 (Integer spectrum). The operator $N$ has no eigenvector out of $\mathbb{N}$.
Proof. Assume that $\lambda \notin \mathbb{N}$ is an eigenvalue of $N$ associated with the eigenvector $\psi_{\lambda} \neq 0$. Since $N=a^{*} a$ is positive, we have necessarily $\lambda>0$. From (1.11), we find that

$$
N a \psi_{\lambda}=[N, a] \psi_{\lambda}+a N \psi_{\lambda}=(\lambda-1) a \psi_{\lambda} .
$$

We know that $a \psi_{\lambda} \neq 0$ otherwise $\psi_{\lambda}=C \psi_{0}$ so that $\lambda=0$ which is a contradiction. We can iterate this argument.
An3: The above proof requires to know that the successive $a \psi_{\lambda}, a^{2} \psi_{\lambda}, \cdots$ are indeed in the domain of $a$. Again, this hypothesis (which is viewed here as being implicitly satisfied) can easily be verified by analysis.
The vector $a^{m} \psi_{\lambda}$ with $m=\lfloor\lambda\rfloor+1$ furnishes an eigenvector associated with the eigenvalue $\lambda-m$ with (since $\lambda$ is not an integer) the bounds $-1<\lambda-m<0$. The existence of such negative eigenvector is a contradiction.

The map $a$ is called the lowering operator because (as shown above) it allows to go one step back in energy. Starting from $\psi_{n}$, we can return to the fundamental state after $n$ iterations ( $a^{n} \psi_{n} \sim \psi_{0}$ ). Then, this leads to the zero vector (since $a^{m} \psi_{n}=0$ for $m>n$ ).


Lemma 8. All the (integer) eigenvalues of $N$ are of multiplicity one.
Proof. For $n=0$, the dimension of the kernel of $N$ is 1 due to the assumption (1.9). Suppose that the dimension of $\operatorname{ker}(N-j I d)$ is 1 for all $j \leq n$, that is:

$$
\forall j \in\{0, \cdots, n\}, \quad \operatorname{ker}(N-j I d)=\left\{C \psi_{j} ; C \in \mathbb{C}\right\} .
$$

Let $\psi$ be an eigenvector of $N$ associated with the eigenvalue $n+1$. We have just seen that $a \psi$ is an eigenvector associated to the eigenvalue $n$, and it is therefore of the form $a \psi=C \psi_{n}$. We apply $c$ to recover:

$$
c a \psi=N \psi=(n+1) \psi=C c \psi_{n}=C \psi_{n+1},
$$

which shows that $\psi$ must be colinear to $\psi_{n+1}$.

Remark 9. The action of $c, a, N$ and $H$ viewed in terms of matrices, that is according to the viewpoint of Heisenberg, is developped in [2]-paragraph 5.1.4. The eigenfunctions of a which are called états cohérents are described in [2]-part 5.2.

At this stage, we have an exhaustive description of the point spectrum $\sigma_{p}(H)$ of $H$. We know that $\sigma_{p}(H) \subset \sigma(H)$. But do we have $\sigma_{p}(H)=\sigma(H)$ ?
Let $G$ be the closure of the vector space spanned by the $\psi_{n}$. If $G=\mathcal{H}$, its over. Otherwise, by construction, the space $G$ is stable by $a$ and $a^{*}$. Its orthogonal complement $G^{\perp}$ is invariant under the action of $a^{*}$ and $a$, and thereby under the action of $N=a^{*} a$. We can therefore consider the restriction of $N$ to $G^{\perp}$, and repeat the preceding procedure. This argument faces (again) domain considerations. Furthermore, we do not have necessarily for $N_{\mid G^{\perp}}$ some initiation step of the type (1.9). To complete our study, some analytical arguments are needed.
1.3. The analytical approach. That means to look at

$$
H=-\partial_{q}^{2}+q^{2}, \quad \mathcal{H}=L^{2}(\mathbb{R}) .
$$

This allows to fill in the gaps mentioned above. This gives access to a more concrete intuition. By this way, we can also develop further perspectives
Since $H$ is of compact resolvant [1], we can directly say that the spectrum of $H$ is discret and built on a sequence of eigenvalues $\lambda_{n}$ which go to $+\infty$. Those are the $\lambda_{n}=n+(1 / 2)$. We now have to show that the $\psi_{n}$ for $n \in \mathbb{N}^{*}$ form a basis of $L^{2}(\mathbb{R})$. The proof is detailed in [1]-paragraph 6.2.2. It is not reproduced here.
1.4. Additional information. The purpose of this paragraph is to furnish development paths:

- The Hermite functions $\psi_{n}$ are drawn in [2]-figure 5.1;
- The reference [3] allows to better understand why it is so useful to represent quantum mechanics in the phase space. It also furnishes through some modeling an intuition about various phenomena such as: the spreading of the wave function (due to dispersion), the quantum tunnelling or the quantum chaos;
- The vectors $\psi_{n}$ play a crucial role from the viewpoint of the Fourier transform $\mathcal{F}$. Indeed, they allow to diagonalize the action of $\mathcal{F}$ according to $\mathcal{F}\left(\psi_{n}\right)=i^{n} \psi_{n}$. This can be seen at the level of the Bargmann transform (or how to see $L^{2}$ as a space of analytic functions).
- The quantum field theory (QFT) describes the evolution of particles, while incorporating the possibility of creation or annihilation in the interaction process. To this end, it implies fields which are operator valued. The field part satisfies propagation equations (of wave, Dirac, ... types). The operator part deals with creation and annihilation. To take into account the possible existence of an infinite number of quantum particles satisfying rules of symmetry (for bosons) or of skewsymmetry (for fermions), we imply a Second quantization. The ladder operators are seen as acting on Fock spaces. The article of P. A. M. Dirac published in 1949 (Annales of IHP) presents the basic ideas as well as fundamental results.


## 2. A step towards quantum electrodynamics (QED)

We have sufficient material to describe (partially) the ideas allowing to pass from a classical description of the electromagnetic field to its quantum conception.
2.0.1. Maxwell's equations. These equations have been proposed in 1861 by J. C. Maxwell. The electric field $\mathbf{E}(t, x)$ is a vector of $\mathbb{R}^{3}$ whose evolution (in vacuum) are driven by the following wave equation (where $c$ is the speed of light):

$$
\begin{equation*}
\left(\partial_{t t}^{2}-c^{2} \Delta_{x}\right) \mathbf{E}=0 . \tag{2.1}
\end{equation*}
$$

Remark 10 (First quantization). The Schrödinger equation is not suitable from a relativistic viewpoint (even if $V \equiv 0$ ), because it is not invariant under the Lorentz group. In special relativity, we work with the four-vector $(E, p)$ whose norm in the Lorentz metric to reveal the rest mass of particles. This gives rise to the dispersion relation which links the energy $E$ to the impulsion $p$ according to:

$$
E^{2}=p^{2} c^{2}+m^{2} c^{4}
$$

Another approach is to write the "Schrödinger equation" that is associated with this new hamiltonian. It is obtained through a (first) quantization replacing $E$ and $p$ by their corresponding observables (which are $-i \hbar \partial_{t}$ and $-i \partial_{x}$ ) leading to the Klein-Gordon equation:

$$
\left(\partial_{t t}^{2}-c^{2} \Delta_{x}+\left(m^{2} c^{4} / \hbar^{2}\right)\right) \psi=0
$$

For $m=0$ (as in the case of photons), if we consider the wave function $\psi$ as a real scalar field propagating in vacuum, we recover (2.1).
Given a direction $k \in \mathbb{R}^{3}$, we can seek solutions of (2.1) in the form of plane waves, that is

$$
\mathbf{E}(t, x)=g(\omega t-k \cdot x), \quad g \in \mathcal{C}^{\infty}\left(\mathbb{R} ; \mathbb{R}^{3}\right)
$$

After substitution, this yields the dispersion relation

$$
\omega(k)= \pm c|k| .
$$

The Gauss's law gives moreover

$$
\operatorname{div} \mathbf{E}=-k \cdot g^{\prime}(\omega t-k \cdot x)=0
$$

which means that $g^{\prime}$ is in a direction belonging to the plane which is orthogonal to $k$, and we can select an orthonormal basis $\left(e_{1}, e_{2}\right)$ of it. Thus, modulo a constant, we have

$$
g(z)=g_{1}(z) e_{1}+g_{2}(z) e_{2}, \quad g_{i} \in \mathcal{C}^{\infty}(\mathbb{R} ; \mathbb{R})
$$

For a wave trapped in a box, we can perform a discrete Fourier analysis. Otherwise, we use the global Fourier transform. By this way, we can decompose the $g_{i}$ as sums of cosinus and sinus. We find building blocks like

$$
\begin{equation*}
g_{1}=E \cos (\omega(k) t-k \cdot x), \quad g_{2}= \pm E \sin (\omega(k) t-k \cdot x) \tag{2.2}
\end{equation*}
$$

where the scalar $E \in \mathbb{R}_{+}$plays the part of an energy, whereas the sign $\pm$is for a right $(+)$and left ( - ). polarization. The different form of polarization are detailed (with pictures) in this text and the mecanisms of superposition of waves are explained in this link. For a photon, there are two possible helicities which correspond to the two possible states of circular polarisation of the photon (clockwise + and counterclockwise -) and they appear after projection of a quantum observable (the spin).
Th wave dynamic (2.2) is the one of a circular motion with radius $E$. The classical electromagnetic radiation in vacuum is therefore equivalent to the sum indexed by $k$ (wave vector) of classical harmonic oscillators that should be doubled due to the helicity ( $\pm$ ). By this way, we get the classical phase space

$$
2 \bigoplus_{k \in \mathbb{R}^{3}} \mathbb{R}_{p_{k}, q_{k}}^{2}
$$

with for each value of $k$ the classical hamiltonian $\left(p_{k}^{2}+\omega(k)^{2} q_{k}^{2}\right) / 2$. More precisely, the idea is not to allow all energies $E$ by replacing this description with its quantum version. At the end, The quantum space $\mathcal{H}$ and its hamiltonian $H$ are respectively

$$
\mathcal{H}=\bigotimes_{k \in \mathbb{R}^{3}}\left(L^{2}\left(\mathbb{R}_{q_{k}}\right) \otimes \mathbb{C}^{2}\right), \quad H=\sum_{k \in \mathbb{R}^{3}} \frac{1}{2}\left(-\partial_{q_{k}}^{2}+\omega(k)^{2} q_{k}^{2}\right),
$$

where $\mathbb{C}^{2}$ is introduced to take into account the spin $(1 / 2)$ of the electron (or its polarisation state). There are other (not mentionned) complications due to the simultaneous presence of many photons as well as their creation and annihilation (this is the second quantifization).

## 3. References

- For an analytic presentation (dealing with questions of domains), see:
[1] C. Cheverry et N. Raymond, A Guide to Spectral Theory: Applications and Exercises, paragraphs 2.6.3 et 6.2;
- For a discussion which makes a comparison with the classical case and then which gives a description of coherent states, see:
[2] R. A. Bertlmann, Theoretical Physics T2, Quantum Mechanics, chapter 5;
- For a comparison of classical and quantum dynamics, see:
[3] F. Faure, films d'animation;
- For a description of applications:
[4] F. Faure, Notes de cours sur la mécanique quantique (chap. 2);
- For useful complements on the spectral study of the Laplacian with various boundary conditions, see:
[5] M. Lewin, Eléments de théorie spectrale: le Laplacien sur un ouvert borné.

