Chapter 1
General Phenomenology of the Quantum World and Elementary Formalism

We quickly review in this chapter the most relevant common features of quantum systems. Readers interested in a concise introduction to the physics of Quantum Mechanics (QM) will profit from [SaTu94]: putting aside the mathematical rigour, it discusses Dirac's formulation of QM from a modern and smart perspective. Here the intention is to formalize in a simple way the ideas that will be developed in full in the subsequent chapters, after introducing the appropriate tools.

1.1 The Physics of Quantum Systems

This first section focuses on phenomenological aspects of quantum systems: in particular, when a physical system can be said to have a quantum nature and what are the basic features of this quantum nature.

1.1.1 When Is a Physical System a Quantum System?

Quantum Mechanics can be roughly defined as the physics of the microscopic world (elementary particles, atoms, molecules). This realm is characterized by a universal constant known as **Planck's constant** h. An associated constant—nowadays of more frequent use—is the **reduced Planck constant**

$$\hbar := \frac{h}{2\pi} = 1.054571726 \times 10^{-34}\,\mathrm{J\,s}\,.$$

The physical dimensions of h (or $\hbar$) are those of an *action*, i.e. *energy* $\times$ *time*. A simple but effective check on the appropriateness of a quantum physical description of the physical system under consideration consists in comparing the

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value of a characteristic action of the system with $\hbar$. Let us consider two examples. First take a macroscopic pendulum (of length, say, $\sim$1 m, mass $\sim$1 kg, maximum speed $\sim 1\,\mathrm{ms}^{-1}$). By multiplying the maximum kinetic energy by the period of the oscillations we find a typical action of roughly $2\,\mathrm{J\,s} \gg \mathrm{h}$. In this situation, quantum physics is definitely inappropriate, an expectation that is matched by our day-to-day experience. If instead we look at a hydrogen atom, the first *ionization energy* of the electron orbiting its proton multiplied the orbital period of rotation gives (using the classical formula with radius of order of 1 Å) a typical action comparable to h. Here Quantum Mechanics is necessary.

1.1.2 Basic Properties of Quantum Systems

A triple of features specific to Quantum Mechanics (QM), which seem to be very different from properties of Classical Mechanics (CM), is listed below. These remarkable general properties concern the physical quantities of physical systems. In QM physical quantities are called *observables*.

(1) **Randomness**. If we measure an observable of a quantum system, the outcomes appear to be *stochastic*: when measuring the same observable A on completely identical systems prepared in the *same* physical state, one generally finds different outcomes $a, a', a'' \ldots$.

If we refer to the standard interpretation of the formalism of QM (see [SEP] for a nice up-to-date account on the various interpretations), this randomness of measurement outcome should not be ascribed to an incomplete knowledge of the state of the system, as happens, for instance, in Classical Statistical Mechanics. Randomness, rather than *epistemic*, is *ontological*, and as such it is a fundamental property of quantum systems.

On the other hand, *QM allows to compute the* probability distribution *of all the outcomes of a given observable, once the state of the system is known*.

Moreover, it is always possible to prepare a state ψ_a in which a certain observable A is *defined* and where it takes the value a. That is, repeated measurements of A give rise to the same value a with probability 1. (Note that we can perform simultaneous measurements on identical systems all prepared in state ψ_a, or we can perform different subsequent measurements on the same system in state ψ_a. In the latter case these measurements have to be performed in rapid succession to prevent the system's state from evolving under Schrödinger evolution, see (3) below.) States where observables take definite values cannot be prepared for *all* observables simultaneously, as discussed in (2).

(2) **Compatible and Incompatible Observables**. The second standout feature of QM is the existence of *incompatible observables*. In contrast to CM, there are physical quantities which cannot be measured simultaneously since there is no physical instrument capable of such a task. If an observable A is *defined* in a

given state ψ—i.e. it attains a precise value a with probability 1 if measured—an observable B *incompatible* with A turns out to be *not defined* in the state ψ: it may attain *several different* values $b, b', b'' \ldots$, *none with probability* 1, in case of measurement. So, if we measure B we generally obtain a spectrum of values described by a distribution of frequencies, as mentioned in (1), by identifying the frequencies with corresponding a priori probabilities.

Incompatibility is *symmetric*: A is incompatible with B if and only if B is incompatible with A, though it is not *transitive*.

Compatible observables do exist and, by definition, they can be measured simultaneously. The component x of the position of a particle and the component y of its momentum are an example, if we refer to the rest space of a given inertial reference frame.

A popular instance of incompatible observables are pairs of *canonically conjugate observables*, like the position X and the momentum P of a particle along the same fixed axis of a reference frame. There is a lower bound for the product of the standard deviations—resp. ΔX_ψ, ΔP_ψ—for the outcomes of the measurements of these observables in a given state ψ. These measurements have to be performed on different identical systems all prepared in the same state ψ. The lower bound is independent of the state, and is encoded in the celebrated formula (a theorem in modern formulations)

$$\Delta X_\psi \, \Delta P_\psi \geq \hbar/2 \,, \tag{1.1}$$

which contains the Planck constant.

(3) **Collapse of the State**. Measurements of QM *usually change the state of the system* and give rise to a *post-measurement state* other that the state in which the measurement is performed. (We are considering rather idealized measurement procedures, which tend to be very often destructive.) Assuming ψ is the initial state, immediately after the measurement of an observable A that returns value a among a plethora of possible values $a, a', a'', \ldots$, the state settles in state ψ', in general different form ψ. Relative to ψ', the probabilities of the outcomes of A change to 1 for value a and 0 for all other values. In this sense A becomes *defined* in state ψ'.

If we measure a pair of incompatible observables A, B in alternation and repeatedly, the outcomes will interfere with each other: if the first outcome of A is a, after a measurement of B a subsequent measurement of A gives $a' \neq a$ in general. Instead, if A and B are compatible, the outcomes of subsequent measurements do not disturb one other.

Beside that, in CM there are measurements that, in practice, perturb and are perturbed by the state of the system. It is however theoretically possible to tweak this interference so to render it negligible. In QM this is not always possible, as manifested by (1.1).

Two types of time evolution of the state of a system exist in QM. One is due to the dynamics and is encoded in the famous *Schrödinger equation* we shall encounter in a short while. It is nothing but a quantum version of the classical *Hamiltonian evolution* [Erc15]. The other type is the sudden change of the state caused by the measuring procedure of an observable, which we outlined in (3): the *collapse of the state* (or of the *wavefunction*) of the system.

The physical nature of the second type of evolution remains, nowadays still, a source of animated debate in the community of physicists and philosophers of science. Several attempts have been made to reduce state collapse to a dynamical evolution of the whole physical system, including the measuring instruments and the environment by means of *de-coherence processes* [SEP, BGJ00]. None of these approaches seem to be completely satisfactory, however, at least until now [Lan17].

1.2 Elementary Quantum Formalism: The Finite-Dimensional Case

Remark 1.1 Unless said otherwise, we shall adopt a unit system where $\hbar = 1$ throughout the book. ■

We include here a number of technical details to complete the picture. We intend to show how (1)–(3) should be interpreted mathematically in practice (we shall swap (2) and (3) for convenience). A good part of the chapter is meant to justify and expand these ideas, and place them in a sound mathematical background.

In order to simplify, with the exception of Sect. 1.3 we shall indicate by H a *finite-dimensional* complex vector space endowed with a Hermitian scalar product $\langle\cdot|\cdot\rangle$. The linear entry is the second one. Given H, $\mathfrak{B}(\mathsf{H})$ is the complex algebra of operators $A : \mathsf{H} \to \mathsf{H}$. We remind that if $A \in \mathfrak{B}(\mathsf{H})$, H finite-dimensional, the *adjoint operator* $A^* \in \mathfrak{B}(\mathsf{H})$ is the unique linear operator satisfying

$$\langle A^* x|y\rangle = \langle x|Ay\rangle \quad \text{for all} x, y \in \mathsf{H}. \tag{1.2}$$

A is called *selfadjoint* when $A = A^*$. As a consequence,

$$\langle Ax|y\rangle = \langle x|Ay\rangle \quad \text{for all } x, y \in \mathsf{H}. \tag{1.3}$$

As $\langle\cdot|\cdot\rangle$ is linear in the second argument and anti-linear in the first, evidently all eigenvalues of a selfadjoint operator A must be real.

The mathematical axioms describing quantum systems are:

1. a quantum mechanical system S is associated with a (finite-dimensional, for now) complex vector space H endowed with a Hermitian scalar product $\langle\cdot|\cdot\rangle$;
2. observables are described by *selfadjoint* operators A on H;
3. states are equivalence classes of *unit* vectors $\psi \in \mathsf{H}$, with $\psi \sim \psi'$ iff $\psi = e^{ia}\psi'$ for some $a \in \mathbb{R}$.

Remark 1.2

(a) States are therefore in one-to-one correspondence to elements of the *complex projective space* $P\mathsf{H}$. The states we consider in this introduction are actually called *pure* states. A more general notion will be introduced later.
(b) H is a very simple instance of a complex Hilbert space: it is automatically complete in view of its finite-dimensionality.
(c) Since $\dim(\mathsf{H}) < +\infty$, every selfadjoint operator $A \in \mathfrak{B}(\mathsf{H})$ admits a spectral decomposition

$$A = \sum_{a \in \sigma(A)} a P_a^{(A)} , \tag{1.4}$$

where $\sigma(A)$ is the *finite* set of eigenvalues, which must be *real* as A is selfadjoint, and $P_a^{(A)}$ is the orthogonal projector onto the a-eigenspace. Note that $P_a P_{a'} = 0$ if $a \neq a'$, for eigenvectors with different eigenvalues are orthogonal. ■

Let us see how assumptions 1–3 allow to phrase the physical properties of quantum systems (1)–(3) in mathematically solid form.

(1) Randomness The eigenvalues of an observable A are interpreted physically as the possible values of the outcomes of a measurement of A.

Given a state, represented by the unit vector $\psi \in \mathsf{H}$, the probability to obtain $a \in \sigma(A)$ for A is

$$\mu_\psi^{(A)}(a) := ||P_a^{(A)}\psi||^2 .$$

Going along with this interpretation, the expectation value of A in state ψ is

$$\langle A \rangle_\psi := \sum_{a \in \sigma(A)} a \mu_\psi^{(A)}(a) = \langle \psi | A\psi \rangle .$$

Hence

$$\langle A \rangle_\psi = \langle \psi | A\psi \rangle . \tag{1.5}$$

Similarly, the standard deviation ΔA_ψ turns out to be

$$\Delta A_\psi^2 := \sum_{a \in \sigma(A)} (a - \langle A \rangle_\psi)^2 \mu_\psi^{(A)}(a) = \langle \psi | A^2 \psi \rangle - \langle \psi | A\psi \rangle^2 . \tag{1.6}$$

Remark 1.3

(a) We emphasize that the phase of a unit vector $\psi \in \mathsf{H}$ ($e^{ia}\psi$ and ψ represent the same quantum state for every $a \in \mathbb{R}$) is actually harmless.
(b) If A is an observable and $f : \mathbb{R} \to \mathbb{R}$ is a given map, $f(A)$ is interpreted as an observable whose values are $f(a)$ if $a \in \sigma(a)$: taking (1.4) into account,

$$f(A) := \sum_{a \in \sigma(A)} f(a) P_a^{(A)} . \tag{1.7}$$

For polynomials $f(x) = \sum_{k=0}^{n} a_k x^k$, we have $f(A) = \sum_{k=0}^{n} a_k A^k$, as expected. The selfadjoint operator A^2 can be interpreted in this way, as the natural observable whose values are a^2 when $a \in \sigma(A)$. Then the last term in (1.6) reads, by taking (1.5) into account,

$$\Delta A_\psi^2 = \langle A^2 \rangle_\psi - \langle A \rangle_\psi^2 = \langle (A - \langle A \rangle_\psi I)^2 \rangle_\psi = \langle \psi | (A - \langle A \rangle_\psi I)^2 \psi \rangle . \tag{1.8}$$

■

(3) Collapse of the State Let a be the outcome of the (idealized) measurement of A when the state is represented by ψ. The post-measurement state is given by the unit vector

$$\psi' := \frac{P_a^{(A)} \psi}{||P_a^{(A)} \psi||} . \tag{1.9}$$

Remark 1.4 The above formula is meaningless if $\mu_\psi^{(A)}(a) = 0$, as it should. Yet, the choice of phase in ψ does not cause trouble due to the linearity of $P_a^{(A)}$.

(2) Compatible and Incompatible Observables Two observables A and B are compatible—i.e. they can be measured simultaneously—if and only if the associated operators *commute*:

$$AB - BA = 0 .$$

Since H has finite dimension, A and B are compatible if and only if the associated spectral projectors commute as well (the proof is elementary):

$$P_a^{(A)} P_b^{(B)} = P_b^{(B)} P_a^{(A)} \quad a \in \sigma(A) , b \in \sigma(B) .$$

In particular,

$$||P_a^{(A)} P_b^{(B)} \psi||^2 = ||P_b^{(B)} P_a^{(A)} \psi||^2$$

has the natural interpretation of the probability to obtain outcomes a and b for a simultaneous measurement of A and B. If, conversely, A and B are incompatible, it may happen that

$$||P_a^{(A)} P_b^{(B)} \psi||^2 \neq ||P_b^{(B)} P_a^{(A)} \psi||^2 .$$

Furthermore, by exploiting (1.9) one can understand

$$||P_a^{(A)} P_b^{(B)} \psi||^2 = \left|\left| P_a^{(A)} \frac{P_b^{(B)} \psi}{||P_b^{(B)} \psi||} \right|\right|^2 ||P_b^{(B)} \psi||^2 \tag{1.10}$$

as *the probability of obtaining first b and then a in successive measurements of B and A*. ■

Remark 1.5

(a) In general the role of A and B in (1.10) cannot be swapped, because $P_a^{(A)} P_b^{(B)} \neq P_b^{(B)} P_a^{(A)}$ when A and B are incompatible. The measurement procedures "interfere with each other", as we saw earlier.
(b) The interpretation of (1.10) as probability of successive measurements is consistent also if A and B are compatible. In that case the probability of obtaining first b and then a in successive measurements of B and A is identical to the probability of measuring a and b simultaneously. In turn, it coincides with the probability of obtaining first a and then b in successive measurements of A and B.
(c) A is always compatible with itself. Moreover $P_a^{(A)} P_a^{(A)} = P_a^{(A)}$, by definition of projector. This fact has the immediate consequence that if we obtain a measuring A so that the state immediately after the measurement is represented by $\psi_a = ||P_a^{(A)} \psi||^{-1} \psi$, it will remain ψ_a even after other measurements of A, and the outcome will always be a. Versions of this phenomenon, especially in relationship to the decay of unstable particles, have been experimentally confirmed and go under the name of *quantum Zeno effect*. ■

Example 1.6 An electron admits a triple of internal observables S_x, S_y, S_z known as the three components of the *spin*. Very roughly speaking, we can think of the spin as the angular momentum of the particle in a moving frame always at rest with the centre of the particle and keeping its axes parallel to the ones of the reference frame of the laboratory where the electron moves. In view of its peculiar properties the spin cannot actually have a complete classical analogue, and this naive interpretation is eventually untenable. For instance, one cannot "stop" the spin of a particle or change the constant value of $S^2 = S_x^2 + S_y^2 + S_z^2$: this quantity is a characteristic property of the particle like the mass. The electron's spin is described by an *internal* Hilbert space H_s, which has dimension 2 so it can be identified with $\mathbb{C}^2$. Up to a constant

factor involving $\hbar$ (depending on conventions), the spin observables

$$S_x = \frac{\hbar}{2}\sigma_x \,, \qquad S_y = \frac{\hbar}{2}\sigma_y \,, \qquad S_z = \frac{\hbar}{2}\sigma_z \,. \tag{1.11}$$

correspond to the well-known *Pauli matrices*

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \,, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \,, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \,. \tag{1.12}$$

Observe that $[S_a, S_b] \neq 0$ if $a \neq b$, implying that the spin's components are incompatible observables. In fact, one has

$$[S_x, S_y] = i\hbar S_z$$

and the similar identities obtained by permuting cyclically the indices. These commutation relations are the same as for the observables L_x,L_y,L_z describing the *angular momentum* in the lab frame, which do possess classical analogues (we shall return to these in Example 7.44). In contrast to CM, the observables describing the angular momenta are incompatible and cannot be measured simultaneously. The failure of compatibility is related to the appearance of $\hbar$ in the right-hand side of

$$[L_x, L_y] = i\hbar L_z \,.$$

That number is extremely small when compared with macroscopic scales. This is the ultimate reason why the incompatibility of L_x and L_z is practically undetectable in macroscopic systems.

Direct inspection proves that $\sigma(S_a) = \{\pm\hbar/2\}$, and similarly $\sigma(L_a) = \{n\hbar \mid n \in \mathbb{Z}\}$. Therefore the components of the angular momentum take discrete values in QM, another difference with CM. Though since the gap between the two nearest values is extremely small if compared to typical angular momenta of macroscopic systems, in practice this discreteness becomes imperceptible and thus disappears. ■

1.2.1 Time Evolution

At this point a few words on time evolution are in order, while we reserve a broader discussion for later.

Among the class of observables of a quantum system described in a given inertial reference frame, the (quantum) *Hamiltonian* H plays a fundamental role. We are assuming that the system interacts with a stationary physical environment and everything refers to the rest space of an inertial system. The one-parameter

group of unitary operators associated with H (see (1.7) for notation)

$$U_t := e^{-itH} := \sum_{h\in\sigma(H)} e^{-ith} P_h^{(H)} , \quad t \in \mathbb{R} \tag{1.13}$$

describes the *time evolution of quantum states*, as follows. Let the state at time $t = 0$ be represented by the unit vector $\psi \in \mathsf{H}$, so at time t the state is represented by

$$\psi_t = U_t \psi .$$

(The vector ψ_t has norm 1 since U_t is unitary and thus preserves norms.) Taking (1.13) into account, this identity is equivalent to

$$i\frac{d\psi_t}{dt} = H\psi_t . \tag{1.14}$$

Equation (1.14) is nothing but a form of the celebrated *Schrödinger equation*. If the environment is not stationary, a more complicated description can be given where H is replaced by a family of (selfadjoint) Hamiltonian operators $H(t)$ parametrised by time $t \in \mathbb{R}$. Time dependence accounts for the evolution in time of the external system interacting with our quantum system. In that case, it is simply assumed that the time evolution of states is again provided by the equation above where H is replaced by $H(t)$:

$$i\frac{d\psi_t}{dt} = H(t)\psi_t . \tag{1.15}$$

This equation permits one to define a two-parameter *groupoid* of unitary operators $U(t_2, t_1)$, where $t_2, t_1 \in \mathbb{R}$, such that

$$\psi_{t_2} = U(t_2, t_1)\psi_{t_1} , \quad t_2, t_1 \in \mathbb{R} .$$

The groupoid structure arises from the following identities: $U(t, t) = I$, $U(t_3, t_2)U(t_2, t_1) = U(t_3, t_2)$ and $U(t_2, t_1)^{-1} = U(t_2, t_1)^* = U(t_1, t_2)$.

In our elementary setup, where H is finite-dimensional, *Dyson's formula* holds

$$U(t_2, t_1) = \sum_{n=0}^{+\infty} \frac{(-i)^n}{n!} \int_{t_1}^{t_2} \cdots \int_{t_1}^{t_2} T[H(\tau_1) \cdots H(\tau_n)]\, d\tau_1 \cdots d\tau_n$$

with the simple hypothesis that the map $\mathbb{R} \ni t \mapsto H_t \in \mathfrak{B}(\mathsf{H})$ is continuous (adopting any topology compatible with the vector-space structure of $\mathfrak{B}(\mathsf{H})$) [Mor18]. In the above formula we set $T[H(\tau_1) \cdots H(\tau_n)] = H(\tau_{\pi(1)}) \cdots H(\tau_\pi(n))$, where the bijective function $\pi : \{1, \ldots, n\} \to \{1, \ldots, n\}$ is a permutation with $\tau_{\pi(1)} \geq \cdots \geq \tau_{\pi(n)}$.

1.3 A First Look at the Infinite-Dimensional Case, CCRs and Quantization Procedures

All the formalism introduced, excluding certain technicalities we shall examine at a later stage, holds also for quantum systems whose complex vector space of states H is *infinite*-dimensional.

To extend the ideas of Sect. 1.2 to the setup where finite-dimensionality is relaxed, it only seems natural to assume that H is complete for the norm $\langle\cdot|\cdot\rangle$. Hence H becomes a *complex Hilbert space*. In particular, completeness ensures the existence of spectral decompositions generalizing (1.4), when referring to *compact* selfadjoint operators.

Notation 1.7 Henceforth $\mathscr{S}(\mathbb{R}^n)$ will denote the vector space of C^∞ complex-valued functions on $\mathbb{R}^n$ which, together with derivatives of all orders in any set of coordinates, decay faster than negative powers of $|x|$ as $|x| \to +\infty$.

From now on $C_c^\infty(\mathbb{R}^n)$ will indicate the vector space of C^∞ complex-valued maps on $\mathbb{R}^n$ with compact support. Finally, $d^n x$ will denote the Lebesgue measure on $\mathbb{R}^n$. ■

1.3.1 The $L^2(\mathbb{R}, dx)$ Model

The simplest example of a quantum system described in an infinite-dimensional Hilbert space is a quantum particle confined to the real line $\mathbb{R}$. In this case, the Hilbert space is $\mathsf{H} := L^2(\mathbb{R}, dx)$, dx denoting the standard Lebesgue measure on $\mathbb{R}$. States are still represented by elements of $P\mathsf{H}$, namely equivalence classes $[\psi]$ of measurable functions $\psi : \mathbb{R} \to \mathbb{C}$ with unit norm, $||[\psi]|| = \int_{\mathbb{R}} |\psi(x)|^2 dx = 1$.

Remark 1.8 Note how we have *two* distinct quotients: ψ and ψ' define the same element $[\psi]$ in $L^2(\mathbb{R}, dx)$ iff $\psi(x) - \psi'(x) \neq 0$ on a set of zero Lebesgue measure. Two unit vectors $[\psi]$ and $[\phi]$ define the same state if $[\psi] = e^{ia}[\phi]$ for some $a \in \mathbb{R}$. ■

Notation 1.9 In the sequel we shall adopt the standard convention of many functional analysis textbooks and denote by ψ, instead of $[\psi]$, the elements of spaces L^2. Tacitly we shall identify functions that differ at most on zero-measure sets. ■

The functions ψ defining states (up to zero-measure sets and phases) are called *wavefunctions*. There is a pair of fundamental observables describing our quantum particle moving in $\mathbb{R}$. One is the *position observable*. The corresponding selfadjoint operator X is the *position operator* defined by

$$(X\psi)(x) := x\psi(x)\,, \quad x \in \mathbb{R}\,, \quad \psi \in L^2(\mathbb{R}, dx)\,.$$

The other observable is the momentum P. Restoring $\hbar$ for the occasion, the *momentum operator* is

$$(P\psi)(x) := -i\hbar\frac{d\psi(x)}{dx}\,, \quad x \in \mathbb{R}\,, \quad \psi \in L^2(\mathbb{R}, dx)\,.$$

We are immediately confronted by a number of mathematical issues with these, actually quite naive, definitions. Let us begin with X. First of all, in general $X\psi \notin L^2(\mathbb{R}, dx)$ even if $\psi \in L^2(\mathbb{R}, dx)$. To fix the problem, one could simply restrict the domain of X to the linear subspace

$$D(X) := \left\{ \psi \in L^2(\mathbb{R}, dx) \;\middle|\; \int_{\mathbb{R}} |x\psi(x)|^2 dx < +\infty \right\}\,. \tag{1.16}$$

Even if

$$\langle X\psi|\phi\rangle = \langle\psi|X\phi\rangle \quad \text{for all } \psi, \phi \in D(X), \tag{1.17}$$

holds, we cannot argue that X is properly selfadjoint because we have *not yet* given the definition of adjoint to an operator defined on a non-maximal domain in an infinite-dimensional Hilbert space. Identity (1.2) in an infinite-dimensional Hilbert space does not define a (unique) operator X^* without further technical requirements. (Readers need not hold their breath, for X is truly selfadjoint on some domain (1.16) according to a general definition, see the next chapter.) From a very practical viewpoint however, (1.17) implies that all the eigenvalues of X, if any, must be real, which seems sufficient to adopt the standard interpretation of eigenvalues as outcomes of measurements of the observable X. Unfortunately life is not as easy: for every fixed $x_0 \in \mathbb{R}$ there is no $\psi \in L^2(\mathbb{R}, dx)$ with $X\psi = x_0\psi$ and $\psi \neq 0$. (A function ψ satisfying $X\psi = x_0\psi$ must also satisfy $\psi(x) = 0$ if $x \neq x_0$, due to the definition of X. Hence $\psi = 0$ in $L^2(\mathbb{R}, dx)$, simply because $\{x_0\}$ has zero Lebesgue measure!)

All this seems to prevent the existence of a spectral decomposition of X like (1.4), since X does not admit eigenvectors in $L^2(\mathbb{R}, dx)$ (and a fortiori in $D(X)$).

The definition of P appears to suffer from even worse problems. Its domain cannot be the whole $L^2(\mathbb{R}, dx)$ but should be a subset of differentiable functions with derivative in $L^2(\mathbb{R}, dx)$. The weakest notion of differentiability we can assume is *weak differentiability*, leading to this candidate for domain

$$D(P) := \left\{ \psi \in L^2(\mathbb{R}, dx) \;\middle|\; \exists\, \text{w-}\frac{d\psi(x)}{dx}\,,\ \int_{\mathbb{R}} \left|\text{w-}\frac{d\psi(x)}{dx}\right|^2 dx < +\infty \right\}\,. \tag{1.18}$$

Above w-$\frac{d\psi(x)}{dx}$ denotes the *weak derivative* of ψ.[1] As a matter of fact $D(P)$ coincides with the *Sobolev space* $H^1(\mathbb{R})$.

Again, without a precise definition of adjoint on an infinite-dimensional Hilbert space (with non-maximal domain) we cannot say anything more precise about the selfadjointness of P with that domain. (As before P will turn out to be selfadjoint under the general definition we shall give in the next chapter.)

Passing to the Fourier-Plancherel transform, one finds (some work is needed)

$$\langle P\psi|\phi\rangle = \langle\psi|P\phi\rangle \quad \text{for all } \psi, \phi \in D(P), \tag{1.19}$$

so that eigenvalues are real provided they exist. Exactly as we saw for X, neither P admits eigenvectors. The naive eigenvectors with eigenvalue $p \in \mathbb{R}$ are functions proportional to the map $\mathbb{R} \ni x \mapsto e^{ipx/\hbar}$, which does not belong to $L^2(\mathbb{R}, dx)$ nor $D(P)$. We will tackle these issues in the next chapter in a very general fashion.

Remark 1.10

(a) The space of *Schwartz functions* $\mathscr{S}(\mathbb{R})$ satisfies

$$\mathscr{S}(\mathbb{R}) \subset D(X) \cap D(P),$$

and furthermore $\mathscr{S}(\mathbb{R})$ is dense in $L^2(\mathbb{R}, dx)$ and *invariant* under X and P: $X(\mathscr{S}(\mathbb{R})) \subset \mathscr{S}(\mathbb{R})$ and $P(\mathscr{S}(\mathbb{R})) \subset \mathscr{S}(\mathbb{R})$. This observation has many technical consequences that will resurface elsewhere.

(b) Although we shall not pursue the following, we stress that X admits a set of eigenvectors if we enlarge the domain of X to the space $\mathscr{S}'(\mathbb{R})$ of *Schwartz distributions* in a standard way, taking (a) into account. If $T \in \mathscr{S}'(\mathbb{R})$,

$$\langle X(T), f\rangle := \langle T, X(f)\rangle \quad \text{for every } f \in \mathscr{S}(\mathbb{R}).$$

Thus the eigenvectors in $\mathscr{S}'(\mathbb{R})$ of X with eigenvalue $x_0 \in \mathbb{R}$ are the distributions $c\delta(x - x_0)$. This class of eigenvectors can be exploited to build a spectral decomposition of X similar to (1.4).

Using the same procedure P admits eigenvectors in $\mathscr{S}'(\mathbb{R})$, which are just the above exponential functions. As before, these eigenvectors allow to construct a spectral decomposition of P akin to (1.4). This procedure's core idea can be traced back to Dirac [Dir30], and in fact some 10 years later Schwartz established the *theory of distributions*. The modern construction of spectral decompositions of selfadjoint operators was developed by Gelfand using *rigged Hilbert spaces* [GeVi64]. ■

[1] $f : \mathbb{R} \to \mathbb{C}$, defined up to zero-measure sets, is the weak derivative of $g \in L^2(\mathbb{R}, dx)$ if $\int_{\mathbb{R}} g\frac{dh}{dx}dx = -\int_{\mathbb{R}} fhdx$ for every $h \in C_c^\infty(\mathbb{R})$. If g is differentiable, its standard derivative coincides with the weak one.

1.3.2 The $L^2(\mathbb{R}^n, d^n x)$ Model and Heisenberg's Inequalities

Consider a quantum particle moving in $\mathbb{R}^n$ with Hilbert space $L^2(\mathbb{R}^n, d^n x)$. Introduce observables X_k and P_k representing position and momentum with respect to the k-th axis, $k = 1, 2, \ldots, n$. These operators, which are defined in analogy to the case $n = 1$, have smaller domains than the full Hilbert space. We shall do not recall the domains' expressions (on which the operators turn out to be properly selfadjoint, see the definition in the next chapter). Let us just mention that all admit $\mathscr{S}(\mathbb{R}^n)$ as a common invariant subspace of their domains. On it

$$(X_k\psi)(x) = x_k\psi(x)\,, \qquad (P_k\psi)(x) = -i\hbar\frac{\partial\psi(x)}{\partial x_k}\,, \quad \psi \in \mathscr{S}(\mathbb{R}^n) \tag{1.20}$$

and so

$$\langle X_k\psi|\phi\rangle = \langle\psi|X_k\phi\rangle\,, \quad \langle P_k\psi|\phi\rangle = \langle\psi|P_k\phi\rangle \quad \text{for all } \psi, \phi \in \mathscr{S}(\mathbb{R}^n), \tag{1.21}$$

By direct inspection one easily proves that the *canonical commutation relations* (CCRs)

$$[X_h, P_k] = i\hbar\delta_{hk}I\,, \quad [X_h, X_k] = 0\,, \quad [P_h, P_k] = 0 \tag{1.22}$$

hold provided the operators are restricted to $\mathscr{S}(\mathbb{R}^n)$. If A and B have different domains, the *commutator* $[A, B] := AB - BA$ is intended defined where both AB and BA make sense, $\mathscr{S}(\mathbb{R}^n)$ in the case of concern. Assuming that (1.5) and (1.8) are still valid for X_k and P_k and $\psi \in \mathscr{S}(\mathbb{R}^n)$, (1.22) easily leads to the *Heisenberg uncertainty relations*,

$$\Delta X_{k\psi}\Delta P_{k\psi} \geq \frac{\hbar}{2}\,, \quad \text{for } \psi \in \mathscr{S}(\mathbb{R}^n)\,, \quad ||\psi|| = 1\,, \quad k = 1, 2, \ldots, n\,. \tag{1.23}$$

Exercise 1.11

(1) *Derive inequality (1.23) from (1.22), using (1.5) and (1.8).*

Solution Using (1.5), (1.8) and the Cauchy-Schwarz inequality, it is easy to show (we omit the index $_k$ for simplicity)

$$\Delta X_\psi \Delta P_\psi = ||X'\psi||||P'\psi|| \geq |\langle X'\psi|P'\psi\rangle|$$

where $X' := X - \langle X\rangle_\psi I$ and $P' := X - \langle X\rangle_\psi I$. Next notice that

$$|\langle X'\psi|P'\psi\rangle| \geq |Im\langle X'\psi|P'\psi\rangle| = \frac{1}{2}|\langle X'\psi|P'\psi\rangle - \langle P'\psi|X'\psi\rangle|.$$

Taking advantage of (1.21) and the definitions of X' and P', and exploiting (1.22), we obtain

$$|\langle X'\psi|P'\psi\rangle - \langle P'\psi|X'\psi\rangle| = |\langle\psi|(X'P' - P'X')\psi\rangle| = |\langle\psi|(XP - PX)\psi\rangle| = \hbar|\langle\psi|\psi\rangle|$$

Since $\langle\psi|\psi\rangle = ||\psi||^2 = 1$ by hypotheses, (1.23) is proved. Obviously we still have to justify the validity of (1.5) and (1.8) in the infinite-dimensional case. □

(2) *Prove that there exist no operators* X_h, P_k, $h, k = 1, 2, \ldots, n$, *on a finite-dimensional Hilbert space* $\mathsf{H} \neq \{0\}$ *satisfying (1.22).*

Solution Supposing such operators exist, we would have

$$i\delta_{hk}\dim(\mathsf{H}) = tr([X_h, P_k]) = tr(X_h P_k) - tr(P_k X_h) = tr(P_k X_h) - tr(P_k X_h) = 0,$$

and this is not possible for $h = k$ since $\dim(\mathsf{H}) > 0$. □

1.3.3 Failure of Dirac's Quantization and Deformation Quantization Procedure

A philosophically remarkable consequence of the CCRs (1.22) is that they resemble the *classical canonical commutation relations* of the Hamiltonian variables q^h, p_k for the standard *Poisson bracket* $\{\cdot,\cdot\}_P$,

$$\{q^h, p_k\}_P = \delta^h_k\,, \quad \{q^h, q^k\}_P = 0\,, \quad \{p_h, p_k\}_P = 0\,. \tag{1.24}$$

as soon as one identifies $(i\hbar)^{-1}[\cdot,\cdot]$ with $\{\cdot,\cdot\}_P$. This fact, initially noticed by Dirac [Dir30], leads to the idea of "quantization" of a classical Hamiltonian theory [Erc15, Lan17].

In modern language Dirac's procedure goes like this. Start from a classical system described on a symplectic manifold (Γ, ω), for instance $\Gamma := \mathbb{R}^{2n}$ and ω the canonical symplectic form. The (real) Lie algebra $\mathfrak{g} := (C^\infty(\Gamma, \mathbb{R}), \{\cdot,\cdot\}_P)$ with Lie bracket $\{f, g\}_P := \omega(df, dg)$ gives a *Poisson structure*. To "quantize" the system, one seeks a "quantization map" Q associating classical observables $f \in C^\infty(\Gamma, \mathbb{R})$ (or in a Lie subalgebra, e.g. a polynomial algebra if $\Gamma = \mathbb{R}^{2n}$) to quantum observables $Q(f)$, i.e. selfadjoint operators restricted[2] to a common invariant domain $\mathscr{S}$ in some Hilbert space H. The map $Q : f \mapsto Q(f)$ is expected

[2]The restriction should be defined so that it admits a unique selfadjoint extension. A sufficient requirement on $\mathscr{S}$ is that every $Q(f)$ is *essentially selfadjoint* on it, see the next chapter.

to satisfy certain conditions, including

1. injectivity;
2. $\mathbb{R}$-linearity;
3. $Q(1) = I|_{\mathscr{S}}$ (1 being the constant map 1 on Γ);
4. $[Q(f), Q(g)] = i\hbar Q(\{f, g\}_P)$
5. if (Γ, ω) is the standard $\mathbb{R}^{2n}$, then $Q(x_k) = X_k|_{\mathscr{S}}$ and $Q(p_k) = P_k|_{\mathscr{S}}$, $k = 1, 2, \ldots, n$;
6. the image of Q is irreducible (the only operators commuting with all elements of $Q(\mathfrak{g})$ are multiples of I).

Requirements 1, 2 and 4 say that the map $Q : f \mapsto Q(f)$ is an injective Lie-algebra homomorphism transforming $\mathfrak{g}$ in a real Lie algebra of operators with Lie bracket proportional to $i[Q(f), Q(g)]$. This apparently natural set of requirements turns out to be *mathematically contradictory* in view of the various versions of the *Groenewold-van Hove theorem*. See [GGT96] for a reasoned survey on the subject. *Alas the problem persists if we only take a subset of the conditions, and replace* $C^\infty(\Gamma, \mathbb{R})$ *with a smaller subalgebra, for instance polynomials on* $\mathbb{R}^{2n}$. In summary, no quantization map exists if we insist it agree strictly with Dirac's original take. The problem can be overcome within the paradigm of *Deformation Quantization*, where requirement 4 is relaxed and one allows for additional higher powers of $\hbar$ in the right-hand side. Everything relies upon an associative but *non-commutative quantum product* $*_\hbar : C^\infty(\Gamma, \mathbb{R}) \times C^\infty(\Gamma, \mathbb{R}) \to C^\infty(\Gamma, \mathbb{R})$ encoding all quantum properties already on $C^\infty(\Gamma, \mathbb{R})$. Furthermore, the commutator associated with $*_\hbar$ is supposed to coincide with the commutator of operators under the quantization map. The latter does not add further quantum properties to the game, since everything is already included in $*_\hbar$; it just identifies elements of the quantum (non-commutative) structure $(C^\infty(\Gamma, \mathbb{R}), *_\hbar)$ with operators in a suitable (and in a sense unnecessary) Hilbert space:

$$[Q(f), Q(g)] = Q(f *_\hbar g - g *_\hbar f)\,.$$

Assuming that $*_\hbar$ can be expanded in powers of $\hbar$, the first-order approximation of the $*_\hbar$-commutator is requested to equal $\{\,,\,\}_P$, hence replacing requirement 4 above with:

$$[Q(f), Q(g)] = Q(f *_\hbar g - g *_\hbar f) = Q(i\hbar\{f, g\}_P + \mathcal{O}(\hbar^2)) = i\hbar Q(\{f, g\}_P) + \mathcal{O}(\hbar^2).$$

This modification proves to be feasible and fruitful. There are other remarkable procedures of "quantization" in the literature, but we shall not insist on them [Erc15, Lan17].

Example 1.12 Consider a spinless particle in $3D$ with mass $m > 0$, whose potential energy is a real function $U \in C^\infty(\mathbb{R}^3)$ with polynomial growth and bounded below. Classically, its Hamiltonian function reads

$$h := \sum_{k=1}^{3} \frac{p_k^2}{2m} + U(x) \, .$$

A brute-force quantization procedure in $L^2(\mathbb{R}^3, d^3x)$ would consist in replacing every classical object with operators. This may just about make sense when there are no ordering ambiguities when translating functions like p^2x, since classically $p^2x = pxp = xp^2$. But the new identities would be false at the quantum level. In our case these problems do not arise, so

$$H := \sum_{k=1}^{3} \frac{P_k^2}{2m} + U \, , \tag{1.25}$$

where $(U\psi)(x) := U(x)\psi(x)$, could be accepted as a first quantum model of the Hamiltonian function of our system. The operator is at least defined on $\mathscr{S}(\mathbb{R}^3)$, where $\langle H\psi|\phi\rangle = \langle\psi|H\phi\rangle$. The existence of selfadjoint extensions is a delicate issue (see [Mor18] and especially [Tes14]) that we shall not address. Taking (1.20) into account, one immediately finds that on $\mathscr{S}(\mathbb{R}^3)$

$$H := -\frac{\hbar^2}{2m}\Delta + U \, ,$$

where Δ is the standard Laplace operator on $\mathbb{R}^n$ ($n = 3$ at present)

$$\Delta = \sum_{k=1}^{n} \frac{\partial^2}{\partial x_k^2} \, . \tag{1.26}$$

If we assume that the equation describing the evolution of the quantum system is still[3] (1.14), we find the known form of Schrödinger's equation,

$$i\hbar \frac{d\psi_t}{dt} = -\frac{\hbar^2}{2m}\Delta\psi_t + U\psi_t \, ,$$

for $\psi_\tau \in \mathscr{S}(\mathbb{R}^3)$ and τ varying in a neighbourhood of t (this requirement may be relaxed). To be very accurate, the meaning of the derivative on the left should be specified. We shall only say that it is computed with respect to the natural topology of $L^2(\mathbb{R}^3, d^3x)$. ■

[3]The factor $\hbar$ has to be added in the left-hand side of (1.14) if our unit system has $\hbar \neq 1$.