An introduction to Quantum Mechanics for mathematicians

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CHAPTER 1

Introduction

1. Origins of Quantum Mechanics

This account is based on the beautiful introduction in the famous textbook of Albert Messiah [**4**]; the interested reader can find a longer description there.

Until around 1900, Classical Theory reigned supreme. The physical world consists of *matter* (corpuscular) and of *radiation* (wave-like behaviour). Let M denote the "phase space", that is, the set of all possible states of the physical system. The evolution between times 0 and T is described by a trajectory $[0, T] \to M$ that satisfies a first-order differential equation, such as Hamilton equation for point particles or Maxwell equations for electromagnetic fields. It was then believed that electromagnetic waves take place in some medium called "ether", which might have been a form of matter. It looked like classical theory could describe the whole physical world.

1887: Mickelson and Morley design a precise experiment in order to measure the velocity of the Earth through ether: the result is surprising, there is no velocity!

This result was upsetting, as the prospect of the Earth carrying ether with it did not see appealing. The concept of ether was totally abandoned in 1905 with Einstein's article on special relativity.

At about the same time, the existence of atoms was being confirmed. Thomson had detected the electron in 1897. Einstein and Smochulowski had explained the Brownian motion using the atomic hypothesis, and had found estimates of Avogadro's number (1905).

1896: Discovery of radioactivity. This is an important step, conceptually, and it is even more important experimentally.

1911: Rutherford studies the scattering of α-particles (i.e. He^{++}) by atoms, thus gaining much more information on the properties of the atoms. These consist of a nucleus and of electrons that "gravitate" around it.

It should be remarked that the Coulomb force $\vec{F} = q\vec{E}$) and the Lorentz force ($\vec{F} = q\vec{v} \times \vec{B}$) for charged particles in electric and magnetic fields were well understood.

1900: Max Planck's theory of blackbody radiation. In order to explain the observed distribution of frequencies, he postulates that the exchange of energy ε_ν between matter and radiation is **quantised**:

$$\varepsilon_\nu = h\nu.$$

Here, ν is the frequency and the new constant h is equal to $6.62 \cdot 10^{-34}$ J·s.

For most physicists, Planck's theory was a "lucky mathematical artifice". But it got further confirmations, notably by Einstein's explanation of the photoelectric effect in 1905 (Einstein got his Nobel prize for this).

1924: The Compton effect, about the scattering of photons by electrons. It is observed that the change in wavelength $\Delta\lambda$ only depends on physical constants and on the angle θ of observation:

$$\Delta\lambda = \tfrac{2h}{mc}\sin^2\tfrac{\theta}{2}.$$

Planck's constant appears again! Compton and Debye showed that this formula can be explained if photons make a single elastic collision with an electron. It confirms Planck's law and the corpuscular nature of light. On the other hand, experiments about diffraction and interference of light shows that its evolution is wave-like. A purely corpuscular theory of light does not work.

There are further intriguing facts, such as the spectra of light emission and absorption of atoms. Hydrogen is characterised by Balmer's formula

$$\nu = \tfrac{me^4}{2\hbar^2}\big(\tfrac{1}{n^2} - \tfrac{1}{m^2}\big),$$

with $m, n \in \mathbb{N}, m > n$. Bohr suggested that atoms have "energy levels", $E_n = -\frac{me^4}{2\hbar^2}\frac{1}{n^2}$, $n \in \mathbb{N}$, in the case of Hydrogen.

1922: The experiment of Stern and Gerlach about atoms carrying magnetic moments ("spins") and moving through a magnetic field. The deviation of the trajectory appears to be *quantised*, which cannot be explained by a classical theory.

1923: De Broglie suggests that matter has also wave-like behaviour (this should be contrasted to Einstein's suggestion that light has also corpuscular behaviour).

This can be summarised by the existence of of a "wave-corpuscle duality.

1927: Experiments on the diffraction of electrons by Davisson and Gerner. Even when electrons are sent one by one, their evolution is wave-like.

The years 1910–1925 correspond to the "Old Quantum Theory" whose central tenets are the "Bohr-Sommerfeld quantisation rules". These are ad hoc hypotheses; they are made in order to fit experimental data and there is some arbitrariness to apply them correctly. They do allow to describe many different experiments in a unified way.

From 1923 to 1927, Heisenberg and Schrödinger formulate the basic setting of Quantum Mechanics. Dirac also made major contributions. Later, the mathematical framework was much enhanced by von Neumann. The influence of Quantum Mechanics on the development of mathematics is huge, it was the main motivation for functional analysis.

2. A short survey of Classical Mechanics

In this survey we choose a mathematical structure that is chosen so that Quantum Mechanics can be seen as a rather natural generalisation. This material is very well presented in Vassili Gelfreich's lecture notes [**2**].

The *state* of a classical particle at time $t \in \mathbb{R}$ is described by its position $q(t)$ and momentum $p(t)$. Let $M \subseteq \mathbb{R}^d \times \mathbb{R}^d$ be the set of all states $\big(q(t), p(t)\big)$. The *energy* of the particle is given by the Hamilton function (or "hamiltonian") $H : M \to \mathbb{R}$. This function, which we assume to be differentiable, determines the evolution through *Hamilton equations*:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{1.1}$$

(As usual, $\dot{q}_i$ denotes the time-derivative of the ith component of $q(t) \in \mathbb{R}^d$.) An important special case is a particle moving in an external potential. With the potential function given by $V : \mathbb{R}^d \to \mathbb{R}$, the hamiltonian is $H(p,q) = \frac{p^2}{2m} + V(q)$. Then $\dot{q}_i = \frac{1}{m}p_i$ and $\dot{p}_i = -\frac{\partial V}{\partial q_i}$, which are Newton equations.

The evolution is described the flow

$$\begin{aligned} G_t :& M \to M \\ & (q_0, p_0) \mapsto \big(q(t), p(t)\big). \end{aligned} \tag{1.2}$$

We expand the formalism so we make a link with differential geometry, and so that it can be suitably extended to a quantum setting. Let us consider the algebra of "observables" $\mathcal{A} = C^\infty(M)$, the set of smooth functions $M \to \mathbb{R}$. It is equipped with pointwise addition and multiplication, so it is indeed an algebra. Rather than looking at the trajectory $\big(q(t), p(t)\big)$, we can consider the evolution of observables. Thus we introduce the evolution operator

$$\begin{aligned} U_t :& \mathcal{A} \to \mathcal{A} \\ & U_t f = f \circ G_t. \end{aligned} \tag{1.3}$$

The evolution operator satisfies the group structure

(i) $U_0 = \mathbb{1}$;
(ii) $U_s U_t = U_{s+t}$, $s, t, \in \mathbb{R}$;
(iii) $U_t^{-1} = U_{-t}$, $t \in \mathbb{R}$.

In addition, we have $U_t fg = U_t f\, U_t g$ for all $f, g \in \mathcal{A}$, so U_t is an automorphism of the algebra $\mathcal{A}$.

We define a **state** to be a normalised, positive, linear functional on M. It can be represented by a probability measure by Riez-Markov theorem. With μ denoting the probability measure, and $\big(q(t), p(t)\big)$ the trajectory with initial conditions (q_0, p_0), the expectation of the observable f at time $t \in \mathbb{R}$ is equal to

$$\int_M f\big(q(t), p(t)\big)\mathrm{d}\mu(q_0, p_0) = \int_M U_t f \mathrm{d}\mu. \tag{1.4}$$

Among the relevant states are the Dirac measures δ_{q_0,p_0} that describes a deterministic state.

We see that the evolution is characterised by $U_t f$. It is then natural to consider the trajectories in $\mathcal{A}$ given by $f_t = U_t f$ where f is a fixed initial observable of $\mathcal{A}$. The evolution equation makes use of the *Poisson bracket*, which is the bilinear map

$\mathcal{A} \times \mathcal{A} \to \mathcal{A}$ defined by

$$\{f, g\} = \sum_{i=1}^{d} \Big(\frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} - \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} \Big). \tag{1.5}$$

The Poisson bracket is antisymmetric and it satisfies

- the product rule: $\big\{f, \{g, h\}\big\} = g\{f, h\} + \{f, g\}h$;
- Jacobi's identity: $\big\{f, \{g, h\}\big\} + \big\{h, \{f, g\}\big\} + \big\{g, \{h, f\}\big\} = 0$.

(Then $\mathcal{A}$ is a Lie algebra.) It follows from Hamilton's equations that the trajectory f_t in $\mathcal{A}$ satisfies the differential equation

$$\tfrac{\mathrm{d}}{\mathrm{d}t} f_t = \{H, f_t\}. \tag{1.6}$$

As we see in the next chapter, the structure of Quantum Mechanics looks similar. The algebra of smooth functions is replaced by an algebra of operators, and the Poisson bracket by commutators. Then the evolution equation for quantum systems, the Schrödinger equation, takes a form reminiscent of Eq. (1.6).

EXERCISE 1.1. *Show that the energy is conserved, that is, $H(q(t), p(t)) = H(q_0, p_0)$ where $(q(t), p(t))$ is the trajectory defined by Hamilton equations and starting at (q_0, p_0).*

EXERCISE 1.2. *Show that the evolution equation for observables, Eq. (1.6), indeed follows from the Hamilton equations (1.1).*

CHAPTER 2

Finite-dimensional quantum systems

The description of a quantum system involves a (complex) Hilbert space and operators on this Hilbert space. The Hilbert space for a quantum particle in physical space is $L^2(\mathbb{R}^3)$; it is infinite-dimensional and many relevant operators are unbounded. Before considering the theory in this case, we look at a simpler setting where the Hilbert space is finite-dimensional; that is, we consider $\mathbb{C}^n$ for some $n \in \mathbb{N}$.

1. Operators on $\mathbb{C}^n$

Let $\varphi, \psi \in \mathbb{C}^n$. The **inner product** is

$$\langle \varphi, \psi \rangle = \sum_{i=1}^{n} \overline{\varphi}_i \psi_i. \tag{2.1}$$

It is linear in the second variable and skew-linear in the first variable.[1] We say that ψ is perpendicular or orthogonal to φ, $\psi \perp \varphi$, if $\langle \psi, \varphi \rangle = 0$. The **norm** of a vector φ is $\|\varphi\| = \sqrt{\langle \varphi, \varphi \rangle}$. A collection of vectors $\{e_i\}_{i=1}^n$ in $\mathbb{C}^n$ is an **orthonormal basis** (or just a **basis**) if $\langle e_i, e_j \rangle = \delta_{i,j}$. Any vector $\varphi \in \mathbb{C}^n$ can be written as

$$\varphi = \sum_{i=1}^{n} \langle e_i, \varphi \rangle e_i. \tag{2.2}$$

An **operator** A is a linear map $\mathbb{C}^n \to \mathbb{C}^n$. The corresponding matrix with respect to the basis $\{e_i\}_{i=1}^n$ is $(A_{i,j})_{1 \le i,j \le n}$ where

$$A_{i,j} = \langle e_i, A e_j \rangle. \tag{2.3}$$

The **norm** of the operator A is

$$\|A\| = \sup_{\varphi \neq 0} \frac{\|A\varphi\|}{\|\varphi\|} = \sup_{\|\varphi\|=1} \|A\varphi\|. \tag{2.4}$$

The **adjoint** of A is the operator A^* such that

$$\langle A^* \varphi, \psi \rangle = \langle \varphi, A\psi \rangle \tag{2.5}$$

for all $\varphi, \psi \in \mathbb{C}^n$. The adjoint always exists and is unique. Its matrix representation is

$$(A^*)_{i,j} = \overline{A_{i,j}}. \tag{2.6}$$

[1] This is the usual convention in physics; one advantage is that linear functionals look nice, $f(x) = \langle f, x \rangle$.

An operator A on a finite-dimensional Hilbert space is **hermitian** or **symmetric** or **self-adjoint** if $A = A^*$. The **trace** and the **determinant** of an operator A can be defined with the help of its matrix representation $(A_{i,j})_{1\leq i,j\leq n}$. Namely

$$\operatorname{Tr} A = \sum_{i=1}^{n} A_{i,i} \tag{2.7}$$

and

$$\det A = \sum_{\sigma\in\mathcal{S}_n} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} A_{i,\sigma(i)}; \tag{2.8}$$

the sum is over permutations of n elements. Trace and determinant do not depend on the choice of the basis. One can check that

$$\operatorname{Tr} AB = \operatorname{Tr} BA, \qquad \det AB = \det A \det B. \tag{2.9}$$

An operator A is **invertible** if there exists an operator A^{-1} such that $AA^{-1} = A^{-1}A = \mathbb{1}$. It is known that A is invertible if and only if $\det A \neq 0$ and that its inverse is unique. An operator U is **unitary** if it is invertible and $U^{-1} = U^*$. Equivalently, U is unitary if and only if $\|U\varphi\| = \|\varphi\|$ for all vectors φ. Any unitary operator can be written as $U = \mathrm{e}^{\mathrm{i}A}$ with A hermitian.

If there exists $\varphi \in \mathbb{C}^n$ and $\lambda \in \mathbb{C}$ such that

$$A\varphi = \lambda\varphi, \tag{2.10}$$

then φ is called an **eigenvector** and λ an **eigenvalue** of A. Some important properties of eigenvalues and eigenvectors:

- An operator A on $\mathbb{C}^n$ has at most n distinct eigenvalues.
- The eigenvalues of a hermitian operator are all real; the eigenvalues of a unitary operator have all modulus 1.
- If $AA^* = A^*A$ (i.e. the operator A is **normal**), there exist eigenvectors that form an orthonormal basis of $\mathbb{C}^n$.

An operator A is **positive-definite**, noted $A \geq 0$, if $\langle\varphi, A\varphi\rangle \geq 0$ for all $\varphi \in \mathbb{C}^n$. One can show that positive-definite operators are necessarily hermitian with nonnegative eigenvalues.

An operator P is a **projector** if $P^2 = P$; it is an **orthogonal projector** if in addition $P = P^*$; its eigenvalues are 0 or 1. Given $\varphi \in \mathbb{C}^n$ with $\|\varphi\| = 1$, the orthogonal projector P_φ onto the one-dimensional subspace spanned by φ is given by

$$P_\varphi\psi = \langle\varphi, \psi\rangle\varphi. \tag{2.11}$$

If A is a normal operator and $(\varphi_i)_{i=1}^n$ is an orthonormal basis of eigenvectors with eigenvalues $(\lambda_i)_{i=1}^n$, then we have

$$A = \sum_{i=1}^{n} \lambda_i P_{\varphi_i}. \tag{2.12}$$

Finally, let us point out that the map

$$\begin{aligned} \mathcal{B}\times\mathcal{B} &\to \mathbb{C} \\ (A, B) &\mapsto \langle A, B\rangle = \operatorname{Tr} A^*B \end{aligned} \tag{2.13}$$

is an **inner product** on $\mathcal{B}$. Its Cauchy-Schwarz inequality is useful.

2. Quantum states

In the review of classical systems, we considered the algebra of observables given by smooth functions on the phase space. In Quantum Mechanics, observables are given by self-adjoint operators on a Hilbert space. Then we let $\mathcal{A}$ denote the vector space of hermitian operators on $\mathbb{C}^n$. The usual product of operator is not a multiplication in $\mathcal{A}$ because $(AB)^* = B^*A^*$ which is not always equal to AB, even when A and B are hermitian. A possibility is to introduce the following multiplication:

$$A \bullet B = \tfrac{1}{2}(AB + BA). \tag{2.14}$$

We are not going to use this product much. Instead, we mainly work with the algebra $\mathcal{B}$ of all operators on $\mathbb{C}^n$, with the usual product. The **commutator** of two operators $A, B \in \mathcal{B}$ is

$$[A, B] = AB - BA. \tag{2.15}$$

For $\alpha, \beta \in \mathbb{C}$ and $A, B, C \in \mathcal{B}$, the commutator satisfies the following properties.

(i) Antisymmetric: $[B, A] = -[A, B]$.
(ii) Bilinear: $[\alpha A + \beta B, C] = \alpha[A, C] + \beta[B, C]$, same with the second variable.
(iii) Product rule: $[A, B \bullet C] = [A, B] \bullet C + B \bullet [A, C]$.
(iv) Jacobi's identity: $\big[A, [B, C]\big] + \big[B, [C, A]\big] + \big[C, [A, B]\big] = 0$

The commutator of hermitian operators is not always hermitian. But we can consider the "quantum Poisson bracket"

$$\{A, B\} = \mathrm{i}[A, B]. \tag{2.16}$$

The quantum Poisson bracket of hermitian operators is hermitian; then $\mathcal{A}$ and $\mathcal{B}$ are Lie algebras.

A state is a real linear functional on the algebra of observables $\mathcal{A}$. But it is more convenient, and is actually equivalent, to consider complex linear functionals on $\mathcal{B}$ (see Exercise 2.2). We then define a **state** to be a map $\omega : \mathcal{B} \to \mathbb{C}$ that is

(i) linear: $\omega(\alpha A + \beta B) = \alpha\omega(A) + \beta\omega(B)$ for all $\alpha, \beta \in \mathbb{C}$ and $A, B \in \mathcal{B}$;
(ii) positive: $\omega(A^*A) \geq 0$ for all $A \in \mathcal{B}$;
(iii) normalised: $\omega(\mathbb{1}) = 1$.

It turns out that states can be represented by density operators, a very useful property. A **density operator** ρ is a positive-definite hermitian operator such that $\operatorname{Tr}\rho = 1$. Given a density operator, there corresponds the state

$$\omega(A) = \operatorname{Tr}\rho A. \tag{2.17}$$

The converse is also true, each state is represented by a density operator.

PROPOSITION 2.1 (Riesz representation of states). *Let ω be a state. Then there exists a unique density operator ρ such that $\omega(A) = \operatorname{Tr}\rho A$ for all $A \in \mathcal{B}$.*

PROOF. Recall the operator inner product defined in (2.13). This inner product turns $\mathcal{B}$ into a Hilbert space. The standard Riesz representation theorem implies that $\mathcal{B}$ is self-dual, that is, every linear functional $\omega : \mathcal{B} \to \mathbb{C}$ is represented by a unique operator ρ such that

$$\omega(A) = \langle \rho, A\rangle = \operatorname{Tr}\rho^* A. \tag{2.18}$$

There remains to check that ρ is a density operator. We have for all $\varphi \in \mathbb{C}^n$ with $\|\varphi\| = 1$ that

$$\langle \varphi, \rho^*\varphi\rangle = \operatorname{Tr} P_\varphi \rho^* = \omega(P_\varphi) = \omega(P_\varphi^2) \geq 0. \tag{2.19}$$

Then ρ^* is positive-definite; it is therefore hermitian so $\rho \geq 0$ as well. Finally, $1 = \omega(\mathbb{1}) = \operatorname{Tr}\rho\mathbb{1}$, so ρ is indeed a density operator. □

The set of states is *convex*: If ω_1, ω_2 are two states, the convex combination $\alpha\omega_1 + (1-\alpha)\omega_2$ is also a state for all $\alpha \in [0,1]$. A state is **mixed** if it can be written as a convex combination of distinct states. A state is **pure** if it is not mixed; in other words, pure states are the extremal points of the convex set of states.

Given $\varphi \in \mathbb{C}^n$, the corresponding projector P_φ is a special case of a density operator, hence it gives a state. It is perhaps expected that this state is pure, and that all pure states are represented by projectors.

PROPOSITION 2.2. *A state is pure if and only if its density operator is equal to P_φ for some $\varphi \in \mathbb{C}^n$.*

PROOF. The density operator ρ of the state is hermitian and it can be written as

$$\rho = \sum_{i=1}^{n} \lambda_i P_{\varphi_i}, \tag{2.20}$$

where the φ_is form a basis of eigenvectors. This can be viewed as a convex combination of density operators. This shows that if ρ is not equal to a projector, then the corresponding state is mixed.

There remains to show that if ρ is a projector, then the state is pure; this takes more efforts. Let $P_\varphi = \rho$ and assume that $P_\varphi = \alpha M + (1-\alpha)N$ with $\alpha \in (0,1)$ and M, N density operators. We want to conclude that M must be equal to N. We progressively show that

(i) $\langle \psi, M\psi\rangle = \langle \psi, N\psi\rangle = 0$ for all $\psi \perp \varphi$.
(ii) $M\psi = N\psi = 0$ for all $\psi \perp \varphi$.
(iii) $M\varphi = N\varphi = \varphi$.

It follows immediately from (ii) and (iii) that M and N are both equal to P_φ.

To obtain (i), we note that $P_\varphi\psi = 0$ if $\psi \perp \varphi$, so that

$$0 = \langle \psi, P_\varphi\psi\rangle = \alpha\langle \psi, M\psi\rangle + (1-\alpha)\langle \psi, N\psi\rangle. \tag{2.21}$$

Since $\langle \psi, M\psi\rangle$ and $\langle \psi, N\psi\rangle$ are nonnegative, they must be zero.

To obtain (ii), let $\psi \perp \varphi$ and $\xi \in \mathbb{C}^n$. For all $\beta \in \mathbb{R}$, we have that

$$0 \leq \langle \beta\psi + \xi, M(\beta\psi + \xi)\rangle = \beta^2\langle \psi, M\psi\rangle + 2\beta \operatorname{Re}\langle \xi, M\psi\rangle + \langle \xi, M\xi\rangle. \tag{2.22}$$

Since $\langle \psi, M\psi\rangle = 0$ by (i), we get $\operatorname{Re}\langle \xi, M\psi\rangle = 0$; replacing ξ by $\mathrm{i}\xi$, we similarly get that $\operatorname{Im}\langle \xi, M\psi\rangle = 0$. Then $\langle \xi, M\psi\rangle = 0$ for all ξ, hence $M\psi = 0$. The same argument obviously applies to N as well.

To obtain (iii), observe that for all $\psi \perp \varphi$, we have

$$\langle \psi, M\varphi\rangle = \langle M\psi, \varphi\rangle = 0. \tag{2.23}$$

Then $M\varphi$ must be equal to $\lambda\varphi$ for some $\lambda \in \mathbb{C}$. In a basis that includes φ, the matrix of M is diagonal and all diagonal values are 0 except for one that is equal to λ. Since $\operatorname{Tr} M = 1$, we get $\lambda = 1$. Same for N. □

Often in Quantum Mechanics, the state of the system is given by a normalised vector φ in $\mathbb{C}^n$ (or in another Hilbert space) and the corresponding expectation of an observable A is $\langle \varphi, A\varphi\rangle$. This is a special case of the above setting; the state corresponding to φ is the pure state with density operator P_φ.

We now discuss the Heisenberg uncertainty principle. It is often formulated for pure states, which is interesting and relevant, but it can be extended to arbitrary states.

Consider an observable A and assume that the system is in the state ω. An experiment can yield many possible values. If the experiment is repeated (with the same initial state ω), the average of the outcomes converges to $\omega(A)$. It is natural to quantify the fluctuations with respect to the average by introducing the **standard deviation** σ_ω, defined by

$$\sigma_\omega(A)^2 = \omega(A^2) - \omega(A)^2 = \omega\big([A - \omega(A)\mathbb{1}]^2\big). \tag{2.24}$$

Classically, there exist states such that the standard deviations are zero for all observables (this corresponds to Dirac measures on the phase space). But this is no longer possible in Quantum Mechanics! This is a consequence of the Heisenberg principle, which gives a lower bound for the standard deviations of two observables, in terms of expectation of their commutator.

THEOREM 2.3 (Heisenberg Uncertainty Principle). *For any state ω on $\mathcal{B}$, and any operators $A, B \in \mathcal{B}$, we have*

$$\sigma_\omega(A)\sigma_\omega(B) \geq \tfrac{1}{2}\big|\omega([A,B])\big|.$$

PROOF. With ρ the density operator of the state ω, we have

$$\big|\omega([A,B])\big| \leq |\operatorname{Tr}\rho AB| + |\operatorname{Tr}\rho BA|. \tag{2.25}$$

Since ρ is positive-definite it has a square-root; using the Cauchy-Schwarz inequality for the operator inner product defined in (2.13), we have

$$|\operatorname{Tr}\rho AB|^2 = |\operatorname{Tr} B\rho^{1/2}\rho^{1/2}A|^2 \leq \operatorname{Tr} B\rho^{1/2}\rho^{1/2}B \operatorname{Tr} A\rho^{1/2}\rho^{1/2}A = \omega(A^2)\omega(B^2). \tag{2.26}$$

The same holds for $\operatorname{Tr}\rho BA$ and we obtain

$$\omega(A^2)\omega(B^2) \geq \tfrac{1}{4}\big|\omega([A,B])\big|^2. \tag{2.27}$$

We can substitute A with $A-\omega(A)\mathbb{1}$ and B with $B-\omega(B)\mathbb{1}$. The left side then involves standard deviations, and the commutator in the right side does not change. □

3. Quantum evolution

We now discuss the equations that govern the dynamics of quantum systems. We first consider the traditional framework of Quantum Mechanics where the possible states are described by unit vectors in a Hilbert space; we take it to be $\mathbb{C}^n$ in this chapter. The evolution to time t is given by a map $U_t : \mathbb{C}^n \to \mathbb{C}^n$ that needs to satisfy the following properties. For all $s,t \in \mathbb{R}$ and $\varphi \in \mathbb{C}^n$,

- U_t is linear;
- $\|U_t\varphi\| = \|\varphi\|$;
- $U_{s+t} = U_sU_t$ and $U_0 = \mathbb{1}$.

The last property means that the laws of motion do not change in time. Then U_t is unitary and it can be written as

$$U_t = \mathrm{e}^{-\mathrm{i}tH} \tag{2.28}$$

for some hermitian operator H. (This can be established using Stone's theorem, that can be found below in a more general context.) Denoting $\varphi_t = U_t\varphi_0$ the vector at time t, we easily check that it satisfies **Schrödinger equation**:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t = H\varphi_t. \tag{2.29}$$

The evolution given by U_t carries over to quantum states. One can check that

$$P_{U_t\varphi} = U_tP_\varphi U_t^*. \tag{2.30}$$

(Indeed, $U_tP_\varphi U_t^*$ is clearly a projector onto some vector of $\mathbb{C}^n$. Then $U_tP_\varphi U_t^*U_t\varphi = U_t\varphi$, so this vector must be to $U_t\varphi$.) The evolution of an arbitrary quantum state follows by linearity. From (2.30), its density operator at time t is given by

$$\rho_t = U_t\rho_0U_t^*. \tag{2.31}$$

The expectation in the state ω_t at time t is then

$$\omega_t(A) = \operatorname{Tr}U_t\rho_0U_t^*A = \operatorname{Tr}\rho_0U_t^*AU_t = \omega_0(U_t^*AU_t). \tag{2.32}$$

If we decide to let the observables evolve rather than the state, we get that $\omega_t(A) = \omega_0(A_t)$ with

$$A_t = U_t^*AU_t. \tag{2.33}$$

The time-dependent operator A_t satisfies the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}A_t = \mathrm{i}[H,A_t]. \tag{2.34}$$

(Check it!) This equation can also be written using the quantum Poisson bracket, namely $\frac{\mathrm{d}}{\mathrm{d}t}A_t = \{H,A_t\}$. This is the same equation as in the classical case! The objects here are operators instead of smooth functions.

It is clear from the equations above that the hermitian operator H plays an important rôle. What is its meaning? Recall Noether's theorem in classical mechanics, that states that to each symmetry there corresponds a conserved observable. This also applies here. Now H is the conserved observable that appears because of time-invariance. By definition, this observable is *the energy*. From now on, we will refer to H as the **hamiltonian**.

A **stationary state** is a state that is invariant over time. Its density operator is constant; since

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = -\mathrm{i}[H,\rho_t] \tag{2.35}$$

(this follows from (2.31)), we see that a state is stationary if and only if its density operator commutes with the hamiltonian.

If the stationary state is pure, i.e. if its density operator is equal to P_φ for some $\varphi \in \mathbb{C}^n$, we have

$$H\varphi = HP_\varphi\varphi = P_\varphi H\varphi. \tag{2.36}$$

Then $H\varphi$ is an eigenvector of P_φ with eigenvalue 1, so $H\varphi = \lambda\varphi$ for some $\lambda \in \mathbb{C}$. This shows that φ is an eigenvector of H (and the eigenvalue λ is real since H is hermitian). Conversely, if the state is given by P_φ with φ an eigenvector of H, then $[H,P_\varphi] = 0$ and the state is stationary. To summarise, the stationary pure states are given by eigenvectors of the hamiltonian.

If the initial state φ_0 is eigenvector of the hamiltonian with eigenvalue λ, $H\varphi_0 = \lambda\varphi_0$, its evolution is given by $\varphi_t = \mathrm{e}^{-\mathrm{i}t\lambda}\varphi_0$. It is not time-invariant, but the corresponding projector P_{φ_t} is. This shows that quantum states are more convenient.

We conclude this chapter with a word on **measurement** in Quantum Mechanics. According to the Copenhagen interpretation, the physical system, initially described by the vector φ_0, evolves deterministically according to the Schrödinger equation until an experiment is performed. To the experiment is associated the observable A (a self-adjoint operator). Assume for simplicity that the spectrum of A only consists of eigenvalues of multiplicity 1. Then the only possible outcomes of the experiment are these eigenvalues; the outcome is random and the probability of measuring the eigenvalue a is $|\langle\varphi_t,\psi_a\rangle|^2$, where φ_t is the vector at time t and ψ_a is the eigenvector of A with eigenvalue a. Further, the state of the system after the experiment if given by ψ_a.

This description is compatible with all experimental observations but it has rattled many physicists ever since it was formulated. Einstein did not like it, who claimed is physically present even nobody is staring at it. There is also an obvious contradiction: Evolution under the Schrödinger equation is smooth, that is, φ_t is continuous in t, but the experiment brings a discontinuity from φ_t to ψ_a. The experiment and its observer can be viewed as a single physical systems whose evolution is given by a Schrödinger equation, and is therefore continuous; there is a contradiction. In recent years physicists have attempted to solve this conundrum with the notion of "decoherence", which purports that large systems have less randomness and more continuity. The debate continues.

EXERCISE 2.1. *Exponential of an operator on* $\mathbb{C}^n$.

(i) *Show that the following Taylor series converges, so it can serve as the definition of* e^A *:*

$$\sum_{k\geq 0} \tfrac{1}{k!} A^k.$$

(ii) *Show that* $(\mathrm{e}^A)^{-1} = \mathrm{e}^{-A}$ *, and that* $\mathrm{e}^A\,\mathrm{e}^B = \mathrm{e}^{A+B}$ *if* $[A,B]=0$.

(iii) *Show that*

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{tA} = A\,\mathrm{e}^{tA}\,.$$

(iv) *Show that if* A *is a normal operator with eigenvectors* $(\varphi_i)_{i=1}^n$ *and corresponding eigenvalues* $(\lambda_i)_{i=1}^n$*, its exponential can be written as*

$$\mathrm{e}^A = \sum_{i=1}^n \mathrm{e}^{\lambda_i}\, P_{\varphi_i}.$$

EXERCISE 2.2. *Let* $\omega : \mathcal{A} \to \mathbb{R}$ *be a (real) linear functional on* $\mathcal{A}$*. Show that there exists a unique extension to a (complex) linear functional* $\hat{\omega} : \mathcal{B} \to \mathbb{C}$*. Hint: An operator can be uniquely decomposed as* $A = B + \mathrm{i}C$ *with* B, C *hermitian; indeed, take* $B = \frac{1}{2}(A^* + A)$ *and* $C = \frac{\mathrm{i}}{2}(A^* - A)$*.*

EXERCISE 2.3. *Give a simpler proof of the Heisenberg Uncertainty Principle (Theorem 2.3) in the case of pure states. The state is given by* $\omega(A) = \langle\varphi, A\varphi\rangle$ *for a* $\varphi \in \mathbb{C}^n$ *and it is enough to invoke the Cauchy-Schwarz inequality in* $\mathbb{C}^n$*.*

CHAPTER 3

Quantum particle in the continuum

1. Square-integrable functions, position and momentum operators

The description of a particle in the continuum involve an infinite-dimensional Hilbert space and is therefore mathematically — and physically — more intricate and interesting.

The state of a quantum particle in $\mathbb{R}^d$ is given by a complex-valued square-integrable function. Let $\mathcal{H} = L^2(\mathbb{R}^d)$ be the Hilbert space of (Lebesgue-) integrable functions with finite L^2 norm:

$$\|f\|^2 = \int_{\mathbb{R}^d} |f(x)|^2 \mathrm{d}x. \tag{3.1}$$

The inner product in $L^2(\mathbb{R}^d)$ is

$$\langle f, g\rangle = \int_{\mathbb{R}^d} \overline{f(x)}\, g(x) \mathrm{d}x. \tag{3.2}$$

As is well-known, $L^2(\mathbb{R}^d)$ is an infinite-dimensional Hilbert space; there exist countable bases (in other words, this Hilbert space is separable). The space C_{c}^∞ of infinitely-many differentiable functions with compact support is dense in $L^2(\mathbb{R}^d)$.

The **Fourier transform** plays a special rôle in quantum mechanics. Let $\mathcal{F}$ be the operator that maps an *integrable* function f to

$$\mathcal{F}f(k) = \widehat{f}(k) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}kx}\, f(x) \mathrm{d}x. \tag{3.3}$$

A remarkable property is that it conserves the L^2 norm, that is, $\|\mathcal{F}f\| = \|f\|$ for all $f \in L^1 \cap L^2$. It is therefore a unitary map, so it is bounded and continuous, and it can be extended by continuity to the whole of $L^2(\mathbb{R}^d)$. If $\widehat{f}$ is an integrable function, the inverse Fourier transform is

$$(\mathcal{F}^{-1}\widehat{f})(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}kx}\, \widehat{f}(k) \mathrm{d}k. \tag{3.4}$$

Since $\mathcal{F}$ is unitary, we have **Plancherel formula**

$$\langle f, g\rangle = \langle \widehat{f}, \widehat{g}\rangle. \tag{3.5}$$

The state of a quantum particle is described by a function $\psi \in L^2(\mathbb{R}^d)$ with norm $|\psi\| = 1$. The *probability density* of finding the particle at $x \in bbR^d$ is equal to $|\psi(x)|^2$ (i.e. the probability of finding the particle in a set $\Lambda \subset \mathbb{R}^d$ is given by $\int_\Lambda |\psi(x)|^2 \mathrm{d}x$). Further, the probability density for the particle to have momentum $k \in \mathbb{R}^d$ is $|\widehat{\psi}(k)|^2$.

We now identify the operators associated with position and momentum. We discuss below a heuristic justification towards the momentum operator.

We simplify the setting that taking $d = 1$; the extension to general d is straightforward. If X denotes the position operator, the average position is equal to $\langle \psi, X\psi\rangle$. It is also given by the expectation with respect to the probability density, so that

$$\langle \psi, X\psi\rangle = \int_{\mathbb{R}} x|\psi(x)|^2 \mathrm{d}x. \tag{3.6}$$

It follows that the position operator is given by the multiplication operator X such that

$$(X\psi)(x) = x\psi(x). \tag{3.7}$$

This presents a mathematical difficulty. While $\psi \in L^2(\mathbb{R})$, the function $x\psi(x)$ is not necessarily square-integrable. This difficulty occurs will all unbounded operators in infinite-dimensional spaces; it is resolved by specifying a **domain** $D(X) \subset L^2(\mathbb{R})$, which is a dense linear subspace of the Hilbert space. Here we can take

$$D(X) = \big\{ f \in L^2(\mathbb{R}) : \int_{\mathbb{R}} x^2 |f(x)|^2 \mathrm{d}x < \infty. \tag{3.8}$$

Then the operator X is a linear map $D(X) \to L^2(\mathbb{R})$. Regarding the momentum, and recalling that $\widehat{\frac{\mathrm{d}}{\mathrm{d}x} f}(k) = \mathrm{i}k\widehat{f}(k)$, the expectation in the state ψ is equal to

$$\int_{\mathbb{R}} k|\widehat{\psi}(k)|^2 \mathrm{d}k = \langle \widehat{\psi}, \widehat{-\mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}x}\psi}\rangle = \langle \psi, -\mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}x}\psi\rangle. \tag{3.9}$$

It follows that the operator associated to the momentum is

$$P = -\mathrm{i}\nabla \tag{3.10}$$

where $\nabla = \frac{\mathrm{d}}{\mathrm{d}x}$. This operator is also unbounded and it should be defined on a domain of functions. For now we can take the space of differentiable functions whose derivative is square-integrable.

We discuss a heuristic for the momentum operator. Let us introduce the **translation operator** T_a, $a \in \mathbb{R}$, by

$$(T_a f)(x) = f(x - a). \tag{3.11}$$

Then $\{T_a\}_{a\in\mathbb{R}}$ is a one-parameter group of unitary operators. By Stone's theorem, there exists a self-adjoint operator P such that

$$T_a = \mathrm{e}^{-\mathrm{i}aP}. \tag{3.12}$$

Conservation of momentum is associated to translation-invariance, so P is the momentum. If f is an analytic function, we have the Taylor series

$$f(x-a) = \sum_{n\geq 0} \frac{(-a)^n}{n!} \frac{\mathrm{d}^n}{\mathrm{d}x^n} f(x) \doteq \mathrm{e}^{-a\frac{\mathrm{d}}{\mathrm{d}x}} f(x). \tag{3.13}$$

Then we indeed have $P = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$. The identity $\doteq$ is mathematically dubious, but it is possible to construct the above objects rigorously, and to establish the identity.

If the particle moves in an external potential, the latter is represented by a **multiplication operator** V. Given a function $V : \mathbb{R} \to \mathbb{R}$, the corresponding multiplication operator is the map

$$\begin{aligned} V :& D(V) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R}) \\ & (Vf)(x) = V(x)f(x). \end{aligned} \tag{3.14}$$

The domain of the operator V must be chosen so that it is dense in $L^2(\mathbb{R})$ and $Vf \in L^2(\mathbb{R})$ for all $f \in D(V)$.

Classically, the energy of a particle in an external potential V is the function $H(q,p) = \frac{1}{2m}p^2 + V(q)$. In Quantum Mechanics, the energy is given by the following **Hamilton operator**, or **hamiltonian**:

$$H = -\Delta + V, \tag{3.15}$$

where $\Delta = \nabla^2 = -P^2$ is the **laplacian**. Notice that we drop all physical constants such as Planck's constant and the mass of the particle; this amounts to a rescaling of space and time.

2. Schrödinger equation

The Schrödinger equation for a quantum particle in an external potential V is

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t) = -\Delta\psi(x,t) + V(x)\psi(x,t), \tag{3.16}$$

with initial condition given by a function $\psi_0(x)$. A solution $\psi(x,t)$ is a **classical solution** if it satisfies the following regularity conditions:

- For each fixed x, $\psi(x,\cdot) \in C^1([0,\infty))$. Further, for each $s > 0$ there exist $\tau > 0$ and $g \in L^1(\mathbb{R})$ (they may depend on s) such that $|\frac{\partial}{\partial t}\psi(x,t)|^2 \leq g(x)$ for all $t \in [s-\tau, s+\tau]$ and all $x \in \mathbb{R}$.
- For each fixed $t \geq 0$, $\psi(\cdot,t) \in C^2(\mathbb{R})$ and $\Delta\psi(\cdot,t) \in L^2(\mathbb{R})$.
- For each fixed $t \geq 0$, $V(\cdot)\psi(\cdot,t) \in L^2(\mathbb{R})$.

We shall see later that classical solutions exist for a large class of potentials V and initial conditions. We now check that the L^2 norm of classical solutions is conserved (so that $|\psi(\cdot)|^2$ is a probability density for all times) and that the evolution deterministic (for given initial conditions the solution is unique).

LEMMA 3.1. *If ψ is a classical solution of the Schrödinger equation, then $\int_{\mathbb{R}} |\psi(x,t)|^2 \mathrm{d}x$ is constant in time.*

PROOF. We have

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}}|\psi(x,t)|^2\mathrm{d}x \overset{(a)}{=} \int_{\mathbb{R}}\frac{\partial}{\partial t}|\psi(x,t)|^2\mathrm{d}x\\
&= \int_{\mathbb{R}}\Big[\frac{\partial}{\partial t}\overline{\psi(x,t)}\,\psi(x,t) + \overline{\psi(x,t)}\frac{\partial}{\partial t}\psi(x,t)\Big]\mathrm{d}x\\
&\overset{(b)}{=} \int_{\mathbb{R}}\Big[-\mathrm{i}\Delta\overline{\psi(x,t)}\,\psi(x,t) + \mathrm{i}V(x)|\psi(x,t)|^2 + \mathrm{i}\overline{\psi(x,t)}\Delta\psi(x,t) - \mathrm{i}V(x)|\psi(x,t)|^2\Big]\mathrm{d}x\\
&\overset{(c)}{=} \mathrm{i}\int_{\mathbb{R}}\Big[\nabla\overline{\psi(x,t)}\,\nabla\psi(x,t) - \nabla\overline{\psi(x,t)}\,\nabla\psi(x,t)\Big]\mathrm{d}x\\
&= 0.
\end{aligned} \tag{3.17}$$

We used (a) e.g. [**1**, Theorem 2.27]; (b) the Schrödinger equation; (c) integration by parts. □

COROLLARY 3.2. *If φ, ψ are two classical solutions of the Schrödinger equation with the same initial condition, i.e. $\varphi(x,0) = \psi(x,0)$ for all $x \in \mathbb{R}$, then $\varphi(x,t) = \psi(x,t)$ for all x, t.*

PROOF. $\varphi - \psi$ is a classical solution and $\int|\varphi(x,0) - \psi(x,0)|^2\mathrm{d}x = 0$. Then $\int|\varphi(x,t) - \psi(x,t)|^2\mathrm{d}x = 0$ for all t by Lemma 3.1, so $\varphi = \psi$. □

The simplest case is the evolution of a free particle, i.e., without external potential ($V = 0$). let $\psi_0(x)$ denote the initial state. We first solve the Schrödinger equation with formal calculations; once we write down the solution, we can verify that it satisfies all properties for being a classical solution.

The Schrödinger equation is $\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t)$. Writing ψ with the help of the inverse Fourier transform, $\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int \mathrm{e}^{\mathrm{i}kx}\,\widehat{\psi}(k,t)\mathrm{d}k$, we get

$$\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\mathrm{e}^{\mathrm{i}kx}\,\mathrm{i}\frac{\partial\widehat{\psi}(k,t)}{\partial t}\mathrm{d}k = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\mathrm{e}^{\mathrm{i}kx}\,k^2\widehat{\psi}(k,t)\mathrm{d}k. \tag{3.18}$$

This must hold for all x, so that $\mathrm{i}\frac{\partial\widehat{\psi}(k,t)}{\partial t} = k^2\widehat{\psi}(k,t)$. The solution is $\widehat{\psi}(k,t) = \mathrm{e}^{-\mathrm{i}k^2t}\,\widehat{\psi}_0(k)$. This allows to write the candidate solution as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\mathrm{e}^{\mathrm{i}kx - \mathrm{i}k^2t}\,\widehat{\psi}_0(k)\mathrm{d}k. \tag{3.19}$$

Under suitable conditions on the initial state ψ_0, e.g. ψ_0 is a Schwartz function, the function above can be seen to be a classical solution. This establishes existence of a solution; uniqueness follows from Corollary 3.2.

The trajectory of a free classical particle is ballistic, that is, it has constant velocity. The quantum counterpart is more complicated. It is not possible to specify an initial condition with fixed position and velocity because of the Heisenberg uncertainty principle (see Theorem 3.4 below). The most classical states are the "wave packets" and they can be shown to have ballistic motion; see Exercise 3.3.

We now consider the *average* motion of a quantum particle in an external potential and shows that it follows the classical equations of motion. This is known as Ehrenfest equations. Given a classical solution $\psi(x,t)$ of the Schrödinger equation (3.16), let

$$\langle A\rangle(t) = \langle\psi(\cdot,t), A\psi(\cdot,t)\rangle \tag{3.20}$$

denote the average of the observable A at time t.

THEOREM 3.3 (Ehrenfest equations). *Let $\psi(x,t)$ be a classical solution of the Schrödinger equation (3.16) such that $\int|\psi(x,t)|^2\mathrm{d}x = 1$, $\int|x|\,|\psi(x,t)|^2\mathrm{d}x < \infty$, and $\int|\nabla V(x)|\,|\psi(x,t)|^2\mathrm{d}x < \infty$. Then*

(i) $\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle(t) = 2\langle P\rangle(t)$.
(ii) $\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle(t) = -\langle\nabla V\rangle(t)$.
(iii) $\frac{\mathrm{d}}{\mathrm{d}t}\langle H\rangle(t) = 0$.

The first two equations are the counterparts of Hamilton's equations — the factor 2 in (i) is present because we have set $2m = 1$. In (ii) the average is taken with respect to the multiplication operator with function ∇V. Notice that the claim (ii) is not straightforward; a natural guess could have been $\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle(t) = -\nabla V(\langle X\rangle(t))$. This theorem is easily extended to higher spatial dimensions.

PROOF. Calculations are essentially straightforward. For (i), we have

$$\begin{aligned}
\tfrac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle(t) &\overset{(a)}{=} \int_{\mathbb{R}} x\big[\tfrac{\partial}{\partial t}\overline{\psi(x,t)}\,\psi(x,t) + \overline{\psi(x,t)}\tfrac{\partial}{\partial t}\psi(x,t)\big]\mathrm{d}x\\
&\overset{(b)}{=} \mathrm{i}\int_{\mathbb{R}}\Big[\nabla\big(x\,\psi(x,t)\big)\nabla\overline{\psi(x,t)} - \nabla\big(x\,\overline{\psi(x,t)}\big)\nabla\psi(x,t)\Big]\mathrm{d}x\\
&= \mathrm{i}\int_{\mathbb{R}}\nabla x\,\big[\nabla\overline{\psi(x,t)}\,\psi(x,t) - \overline{\psi(x,t)}\nabla\psi(x,t)\big]\mathrm{d}x\\
&\overset{(c)}{=} -2\mathrm{i}\int_{\mathbb{R}}\overline{\psi(x,t)}\,\nabla\psi(x,t)\mathrm{d}x\\
&= 2\langle P\rangle(t).
\end{aligned} \tag{3.21}$$

Identity (a) follows e.g. from [**1**, Theorem 2.27]; we get (b) exactly as in the proof of Lemma 3.1, using Schrödinger's equation and integrating by parts; for (c) we integrated by parts and used the fact that $P = -\mathrm{i}\nabla$ is a symmetric operator.

For (ii) the calculations are

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle(t) &= -\mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}} \overline{\psi(x,t)}\,\nabla\psi(x,t)\mathrm{d}x \\ &= -\mathrm{i}\int \big[\tfrac{\partial}{\partial t}\overline{\psi(x,t)}\,\nabla\psi(x,t) + \overline{\psi(x,t)}\nabla\tfrac{\partial}{\partial t}\psi(x,t)\big]\mathrm{d}x \\ &= \dots \\ &= -\int_{\mathbb{R}} \nabla V(x)\,|\psi(x,t)|^2\mathrm{d}x \\ &= -\langle\nabla V\rangle(t).\end{aligned} \tag{3.22}$$

The dots hide the substitution of $\mathrm{i}\frac{\partial}{\partial t}\psi(x,t)$ with $-\Delta\psi(x,t)+V(x)\psi(x,t)$ and integration by parts.

For (iii) we have

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}t}\langle\psi(\cdot,t), H\psi(\cdot,t)\rangle &= \langle\tfrac{\partial}{\partial t}\psi(\cdot,t), H\psi(\cdot,t)\rangle + \langle\psi(\cdot,t), H\tfrac{\partial}{\partial t}\psi(\cdot,t)\rangle \\ &= 2\mathrm{Re}\,\langle H\psi(\cdot,t), \tfrac{\partial}{\partial t}\psi(\cdot,t)\rangle \\ &= -2\mathrm{Re}\,\mathrm{i}\langle H\psi(\cdot,t), H\psi(\cdot,t)\rangle \\ &= 0.\end{aligned} \tag{3.23}$$

We used the assumptions on regularity in order to exchange the order of integration and derivatives; we also used the fact that H is a symmetric operator, which is checked in Exercise 3.1. □

3. Heisenberg Uncertainty Principle

The usual Heisenberg uncertainty principle states that a particle cannot be localised in space and simultaneously have a definite momentum. We present two results. Theorem 3.4 is similar to the one in the finite-dimensional case, Theorem 2.3, while Theorem 3.5 is a bit different. Both results can be viewed as interesting inequalities in Fourier analysis.

THEOREM 3.4 (Heisenberg Uncertainty Principle). *For any $f \in L^2(\mathbb{R})$ with $\|f\| = 1$, and any $x_0, k_0 \in \mathbb{R}$, we have*

$$\int_{\mathbb{R}} (x-x_0)^2|f(x)|^2\mathrm{d}x \int_{\mathbb{R}} (k-k_0)^2|\widehat{f}(k)|^2\mathrm{d}k \geq \frac{1}{4}.$$

Equivalently, we have

$$\|(X-x_0)f\|\cdot\|(P-k_0)f\| \geq \tfrac{1}{2}.$$

This theorem holds in higher spatial dimensions. It quantifies the impossibility to simultaneously localise the wave function in space and momentum. Taking x_0, k_0 to be the average position and momentum, the left side is equal to the product of the squares of the standard deviations. The theorem is optimal in the sense that

the inequality is saturated by gaussian functions, i.e. there is inequality if and only if

$$f(x) = a\,\mathrm{e}^{(x-x_0)k_0}\,\mathrm{e}^{-b(x-x_0)^2} \tag{3.24}$$

with $b > 0$ and $a = \sqrt{b/\pi}$.

PROOF. As in the finite-dimensional version, the proof is based on the Cauchy-Schwarz inequality. We can shift f so that $x_0 = 0$ and add a phase so that $k_0 = 0$. It is then enough to prove that $\|Xf\|\cdot\|Pf\| \geq \frac{1}{2}$ whenever $\|f\| = 1$. Since $[X,P] = \mathrm{i}$, we have

$$\begin{aligned}1 = \langle f, f\rangle &= -\mathrm{i}\langle f, XPf\rangle + \mathrm{i}\langle f, PXf\rangle \\ &= -\mathrm{i}\langle Xf, Pf\rangle + \mathrm{i}\langle Pf, Xf\rangle = 2\mathrm{Re}\,\mathrm{i}\langle Pf, Xf\rangle \\ &\leq 2\|Pf\|\,\|Xf\|.\end{aligned} \tag{3.25}$$

□

In a way, Theorem 3.4 is a special case of Theorem 2.3 with observables A, B such that $[A,B] = c\mathbb{1}$. But such an identity is impossible in finite-dimensional Hilbert space, as can be seen by taking the trace in both sides.

Our second uncertainty principle has some shortcomings — it applies in dimension $d = 1$ only and it does not quite scale correctly. But it is easy to prove and has some nice applications, see Exercise 3.5.

THEOREM 3.5 (Alternate Uncertainty Principle). *For any continuous $f \in L^2(\mathbb{R})$ with $\|f\| = 1$, we have*

$$\sup_{x\in\mathbb{R}} |f(x)|^2 \leq \Big(\int_{\mathbb{R}} k^2|\widehat{f}(k)|^2\mathrm{d}k\Big)^{1/2}.$$

PROOF. By the inverse Fourier transform, we have for any a,

$$f(x) = \frac{1}{\sqrt{2\pi}}\int \sqrt{k^2+a^2}\,\mathrm{e}^{\mathrm{i}kx}\,\widehat{f}(k)\frac{\mathrm{d}k}{\sqrt{k^2+a^2}}. \tag{3.26}$$

Then, using the Cauchy-Schwarz inequality,

$$\begin{aligned}|f(x)|^2 &\leq \frac{1}{2\pi}\Big(\int_{\mathbb{R}}(k^2+a^2)|\widehat{f}(k)|^2\mathrm{d}k\Big)\Big(\int_{\mathbb{R}}\frac{\mathrm{d}k}{k^2+a^2}\Big) \\ &= \frac{1}{2|a|}\int_{\mathbb{R}} k^2|\widehat{f}(k)|^2\mathrm{d}k + \frac{|a|}{2}.\end{aligned} \tag{3.27}$$

The optimal choice is $a^2 = \int_{\mathbb{R}} k^2|\widehat{f}(k)|^2\mathrm{d}k$ and we get the upper bound. □

EXERCISE 3.1. *Check these properties of the position, momentum, and Hamilton operators:*

(i) *they are unbounded, i.e., their operator norms are infinite;*
(ii) *they are symmetric, $\langle f, Xg\rangle = \langle Xf, g\rangle$, same for P and H;*

(iii) *the commutator between X and P is*

$$[X, P] = \mathrm{i}\mathbb{1}. \tag{3.28}$$

Check that $(XP - PX)\psi = \mathrm{i}\psi$ for a set of functions that is dense in $L^2(\mathbb{R})$.

EXERCISE 3.2. *Show that the classical solution of the free particle in Eq. (3.19) can be written as*

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\mathrm{i}t}} \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}(x-y)^2/t}\, \psi_0(y)\mathrm{d}y. \tag{3.29}$$

(Hint: Fubini theorem and gaussian integration.)

EXERCISE 3.3. *Let ψ_0 be a "wave-packet" centred at x_0 with velocity v_0 and standard deviation σ; that is,*

$$\psi_0(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\, \mathrm{e}^{\mathrm{i}v_0(x-x_0)}\, \mathrm{e}^{-(x-x_0)^2/\sigma^2}. \tag{3.30}$$

Show that the classical solution of the free Schrödinger equation with initial condition ψ_0 is

$$\psi(x,t) = \frac{1}{\sqrt{2\pi(\sigma^2 + \mathrm{i}t)}} \exp\Big\{ \frac{(\sigma^2 v_0 + \frac{1}{2}\mathrm{i}(x - x_0))^2}{\sigma^2 + \mathrm{i}t} - \sigma^2 v_0^2 \Big\}. \tag{3.31}$$

Check that the average position is

$$\int_{\mathbb{R}} x|\psi(x,t)|^2 \mathrm{d}x = x_0 + v_0 t; \tag{3.32}$$

this is ballistic motion, as in classical motion! Finally, check that the standard deviation is equal to the square root of

$$\int_{\mathbb{R}} (x - x_0 - v_0 t)^2 |\psi(x,t)|^2 \mathrm{d}x = \sigma^2 + t^2/\sigma^2. \tag{3.33}$$

We observe that the spread of the wave packet increases over time.

EXERCISE 3.4. *Show that both inequalities in Theorem 3.4 are indeed equivalent.*

EXERCISE 3.5. *Give an example of a potential $V : \mathbb{R} \to \mathbb{R}$ that is continuous on $\mathbb{R} \setminus \{0\}$ with $\lim_{x\to 0} V(x) = -\infty$, but such that the hamiltonian $-\Delta + V$ is bounded below.*

This exercise is related to the question of stability of matter: Why is the energy of electrons orbiting a nucleus bounded below, even though the Coulomb potential is not bounded? This prevents us from pumping arbitrarily much energy out of a single atom!

Hint: Use Theorem 3.5 and get a lower bound that involves $\int |V|$, which could be finite.

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