# Topics in Mathematical Physics

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- B. C. Hall. *Quantum Theory for Mathematicians*. Graduate Texts in Mathematics. Volume 267, Springer New York, 2013.
- E. H. Lieb, M. Loss. *Analysis 2*. Second Edition. Graduate Studies in Mathematics. Volume 14, American Mathematical Society.
- E. H. Lieb, R. Seiringer. *The Stability of Matter in Quantum Mechanics*. Cambridge University Press, 2010.
- M. Porta. Lecture notes of a class held at SISSA, Trieste.
- B. Schlein. Lecture notes of a class held at the University of Zurich.

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# 1 Classical Mechanics

## 1.1 One-body Classical Mechanics

*Newton's Equation.* Consider a point particle moving on $\mathbb{R}^d$ at position $x \in \mathbb{R}^d$ with momentum $p \in \mathbb{R}^d$, where $p = mv$, with $m$ the mass and $v = \dot{x}$ the velocity of the particle. The set $\{(x,p) \,|\, (x,p) \in \mathbb{R}^{2d}\}$ of all possible configurations of vectors $(x,p)$ is referred to as the *phase space* of the system. The time evolution of the system is given by the map $t \mapsto (x(t), v(t))$, for all times $t \in \mathbb{R}$. Such map is defined as the solution to the Newton's equation

$$m\ddot{x}(t) = F(x(t)),$$

where $F : \mathbb{R}^d \to \mathbb{R}^d$ is the force field at point $x$. If $F = -\nabla K$, with $K$ a real-valued function called potential, then Newton's equation can be written as

$$\begin{cases} \dot{x}(t) = & p(t)/m, \\ \dot{p}(t) = & -\nabla K(x(t)). \end{cases} \tag{1.1}$$

Observe that, under assumptions on the vector field $(p, -\nabla K) \in \mathbb{R}^d \times \mathbb{R}^d$ (e.g. $(p, -\nabla K) \in \mathrm{Lip}(\mathbb{R}^d)$) there exists a unique solution $(x,p) \in \mathbb{R}^d$ to (1.1) (cfr. standard theory of o.d.e.). In other words, given an initial configuration $(x,p) \in \mathbb{R}^{2d}$ at time $t = 0$, the configuration at time $t > 0$ is uniquely determined by the solution $(x(t), p(t))$ to (1.1), that means that classical mechanics is deterministic.

*Hamiltonian systems.* An important quantity that describes the point particle in the phase space is the Hamiltonian function $\mathcal{H} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

$$\mathcal{H}(x,p) = \frac{p^2}{2m} + K(x), \tag{1.2}$$

whose value represents the *energy* of the system.

**Proposition 1.1.1** (Hamiltonian system)**.** *Given the differentiable Hamiltonian function* (1.2)*, Newton's equation* (1.1) *reads*

$$\begin{cases} \dot{x}(t) = & \frac{\partial \mathcal{H}}{\partial p}(x(t), p(t)), \\ \dot{p}(t) = & -\frac{\partial \mathcal{H}}{\partial x}(x(t), p(t)). \end{cases}$$

*Proof.* The statement follows by direct inspection. □

**Corollary 1.1.2.** *The energy is conserved by the time evolution.*

*Proof.* Proposition 1.1.1 yields

$$\frac{d}{dt}\mathcal{H}(x(t),p(t)) = \frac{\partial \mathcal{H}}{\partial x}\cdot \dot{x}(t) + \frac{\partial \mathcal{H}}{\partial p}\cdot \dot{p}(t) = \frac{\partial \mathcal{H}}{\partial x}\cdot\frac{\partial \mathcal{H}}{\partial p}(x(t),p(t)) - \frac{\partial \mathcal{H}}{\partial p}\cdot\frac{\partial \mathcal{H}}{\partial x}(x(t),p(t)) = 0.$$

Hence the Hamiltonian is preserved by the time-evolution. □

**Definition 1.1.3.** *A (possibly vector-valued) function $A$ defined on the phase space $\mathbb{R}^{2d}$ is called observable.*

**Definition 1.1.4.** *Let $A$ and $B$ be two observables. The Poisson brackets $\{A,B\}$ of $A$ and $B$ are given by*

$$\{A,B\} := \frac{\partial A}{\partial x}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial x}.$$

**Proposition 1.1.5.** *Let $A$ be an observable of the system with Hamiltonian $\mathcal{H}$. The time-evolution of $A$ is given by the Poisson brackets of $A$ and $\mathcal{H}$*

$$\frac{d}{dt}A(x(t),p(t)) = \{A,\mathcal{H}\}(x(t),p(t)).$$

*Proof.* The statement follows by direct inspection. □

**Remark 1.1.6** (Conservation laws)**.** *Every observable $A$ such that $\{A,\mathcal{H}\}=0$ is preserved along the time-evolution. In particular, the conservation of energy follows easily from $\{\mathcal{H},\mathcal{H}\}=0$. In the specific case of a free particle (no force acting on the particle) $\mathcal{H}(x,p) = p^2/2m$ and therefore $\{p,\mathcal{H}\}=0$, which means that momentum is preserved. The importance of conservation laws is due to the fact that they are often the main tool to solve Newton's equation.*

## 1.2 Many-body Classical Mechanics

Most physical systems are made of a big number of particles $N \gg 1$. Let $N$ be the number of particles moving in $\mathbb{R}^d$. A configuration of the system is given by the collection of positions of the $N$ particles $x = (x_1,\dots,x_N) \in \mathbb{R}^{dN}$ and velocities $v = (v_1,\dots,v_N) \in \mathbb{R}^{dN}$. The time evolution of the configuration $(x,v) \in \mathbb{R}^{2dN}$ is given by the system of Newton's equations

$$m_i\ddot{x}_i(t) = F_i(x(t)), \quad i = 1,\dots N,$$

where $m_i$ is the mass of $i$-th particle, and $F_i : \mathbb{R}^{dN} \to \mathbb{R}^d$ is the force acting on particle $i$, which a priori depends on the whole configuration $x \in \mathbb{R}^{dN}$.

*Coulomb potential.* One special interaction in nature is the electrostatic interaction, or Coulomb potential, describing the interaction between two charged particles. To better understand what happens in many-body Coulomb systems, consider $N=2$ and $d=3$. The Coulomb potential then writes $K(x_1,x_2) = q_1q_2/|x_1-x_2|$, where $q_i$ is the charge of particle $i$, $i=1,2$. The corresponding force field $F=(F_1,F_2) \in \mathbb{R}^d \times \mathbb{R}^d$, also called Coulomb force, is given by

$$F_i(x_1,x_2) = -\nabla_{x_i}K(x_1,x_2), \quad K(x_1,x_2) = \frac{q_1q_2}{|x_1-x_2|}, \quad i=1,2.$$

It describes the electrostatic attraction (if $q_1 q_2 < 0$) or repulsion (if $q_1 q_2 > 0$) between two charged particles with charges $q_1$ and $q_2$.
The Hamiltonian associated with such system is

$$\mathcal{H}(x,p) = \sum_{i=1}^{2} \frac{p_i^2}{2m} + \frac{q_1 q_2}{|x_1 - x_2|}.$$

Observe that there are two possible scenarios:

*i)* either $q_1 q_2 > 0$ (i.e. the two particles have charges of the same sign), then the total energy of the system (that is the Hamiltonian) is minimized by taking the particles as much as possible separated. This implies that the electrostatic repulsion prevents the system from forming bound states and the two particles flow away;

*ii)* or $q_1 q_2 < 0$ (i.e. the two particles have opposite signs), then the total energy of the system is minimized when the two particles are close to each other, in such case the Hamiltonian in unbounded below and the system is unstable.

Both situations fail to explain stability of atoms, that are made of neutrons (neutral particles), protons (positively charged particles) and electrons (negatively charged particles). As we shall see, stability of matter finds its rigorous justification in the theory of quantum mechanics.

# 2 Introduction to Quantum Mechanics

## 2.1 Basic Notions

Quantum mechanics is the microscopic theory of nature that describes physics on the scale of atoms and molecules. In analogy with classical mechanics, we will define evolution and observables in quantum mechanics. To this end, we will introduce basic functional analysis notions, which are collected in Appendix A.

*Observables.* Quantum systems are described on Hilbert spaces $\mathcal{H}$ (see Definition A.1.2), that are the analogue of classical mechanic phase spaces. Following the comparison with classical mechanics, states of the system are therefore elements of the Hilbert space, i.e. they are represented by vectors $\psi \in \mathcal{H}$, such that $\|\psi\| = 1$, while observables are associated with self-adjoint operators on $\mathcal{H}$. Here $\|\cdot\|$ denotes the norm induced by the inner product on $\mathcal{H}$. We shall see that $|\psi|^2$ can be interpreted as a probability, making quantum mechanics a non-deterministic theory. It therefore makes sense to consider the expectation of an observable described by the operator $A$ in the state $\psi$ by defining the inner product $\langle \psi, A\psi \rangle$.
In analogy with the classical case, consider a system consisting of a particle moving in $\mathbb{R}^d$, which can be described on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d; \mathbb{C})$ of complex-valued, square integrable functions on $\mathbb{R}^d$. Physically, $|\psi(x)|^2$ is interpreted as the probability density for finding the particle at position $x$. Accordingly, for a measurable set $B \subset \mathbb{R}^d$, the probability that the particle is located in a region $B$ is given by

$$\int_B |\psi(x)|^2 dx = \int \mathbf{1}_B(x) |\psi(x)|^2 dx = \langle \psi, \mathbf{1}_B(x)\psi \rangle$$

where $\mathbf{1}_B$ is the characteristic function of $B$. Similarly, the expectation value of the position of the particle is determined by

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

The function $\psi \in L^2(\mathbb{R}^d)$ is often referred to as the wave function. It does not only determine the distribution of the position of the particle, but also every observable physical quantity is associated with a self-adjoint operator $A$ acting on the Hilbert space $L^2(\mathbb{R}^d)$ so that the expectation value of the observable is given by the inner product $\langle \psi, A\psi \rangle$ and the probability that a measurement of $A$ gives a result in a set $B \subset \mathbb{R}^d$ is determined by $\langle \psi, \mathbf{1}_B(A)\psi \rangle$, where $\mathbf{1}_B(A)$ is defined through functional calculus.

The self-adjoint operator associated with the observable *position of the particle* is the multiplication operator $\psi(x) \mapsto x\psi(x)$. More precisely, for each component $i = 1, \ldots, d$ of the vector $x \in \mathbb{R}^d$, we define the map $\psi(x) \mapsto x_i \psi(x)$ and define the vector made of the $d$ components as the action of the position operator. Notice that the position operator, defined as multiplication through $x$, is an unbounded self-adjoint operator on $L^2(\mathbb{R}^d)$. For this reason, it is not defined on the full Hilbert space $L^2(\mathbb{R}^d)$ but only on the dense subspace consisting of functions $\psi \in L^2(\mathbb{R}^d)$ such that $x\psi(x)$ is again square integrable.

The observable *momentum of the particle* is associated with the self-adjoint operator $p = -i\hbar\nabla$. Notice that also $p$ is a vector-valued observable with components $p_j = -i\hbar\partial_{x_j}$, $j = 1, \ldots, d$ and it is an unbounded self-adjoint operator. Here $\hbar$ is the Planck constant, which we will henceforth assume to be $\hbar = 1$. The expected value of the momentum is therefore given by the expectation

$$\langle \psi, -i\nabla\psi \rangle = -i \int \overline{\psi(x)} \nabla \psi(x) dx$$

Since the Fourier transform diagonalizes the derivative, we can write

$$\langle \psi, -i\nabla\psi \rangle = \int k|\hat{\psi}(k)|^2 dk$$

In other words, $|\hat{\psi}(k)|^2$ is the probability density for finding the momentum close to $k$. This observation explains why it is important for $\psi$ to be complex valued: while $|\psi(x)|^2$ determines the distribution of the position observable, it is the phase of $\psi$, the oscillations of $\psi$, which contributes to $|\hat{\psi}(k)|^2$ and determines the distribution of the momentum observable.

We moreover notice that the position operator is a multiplication operator and its distribution is determined directly by the probability density $|\psi(x)|^2$. The momentum operator is a differential operator, it is diagonal in Fourier space and its distribution is determined by the probability density $|\hat{\psi}(k)|^2$.

For a general self-adjoint operator $A$ on $L^2(\mathbb{R}^d)$, its distribution is determined by the spectral decomposition of $A$. Suppose $\mathcal{H}$ to be finite dimensional. Then we know from Linear Algebra that the spectral theorem holds for self adjoint operators (i.e. symmetric matrices), that is for $A$ self adjoint operator on the finite dimensional space $\mathcal{H}$,

$$A = \sum_j \lambda_j P_{\psi_j}$$

where $\lambda_j \in \mathbb{R}$ are the eigenvalues of $A$ and $P_{\psi_j}$ are orthogonal projections onto the eigenvector $\psi_j$. i.e.

$$P_{\psi_j}\psi = \langle \psi_j, \psi \rangle \psi_j \, .$$

Thus

$$\langle \psi, A\psi \rangle = \sum_j \lambda_j |\langle \psi, \psi_j \rangle|^2.$$

Moreover, by completeness of the orthonormal basis we have $\sum_j |\langle \psi, \psi_j \rangle|^2 = 1$.
Now, if $\mathcal{H}$ is infinite dimensional and $A$ is self adjoint with discrete spectrum, an extension of the spectral theorem holds leading to $A = \sum_j \lambda_j P_{\psi_j}$, $\lambda_j \in \mathbb{R}$ eigenvalues and $P_{\psi_j}$ orthogonal projections onto the eigenvectors $\psi_j$ of $A$. Then, for $\psi \in \mathcal{H}$, $B \subset \mathbb{R}$, we have

$$\begin{aligned} \langle \psi, A\psi \rangle &= \sum_j \lambda_j |\langle \psi, \psi_j \rangle|^2 \\ \langle \psi, \mathbf{1}_B \psi \rangle &= \sum_j \mathbf{1}_B(\lambda_j) |\langle \psi, \psi_j \rangle|^2 = \sum_{j \, : \, \lambda_j \in B} |\langle \psi, \psi_j \rangle|^2 \end{aligned}$$

This means that the observable $A$ takes the values $\lambda_j$ with probability $|\langle \psi, \psi_j \rangle|^2$. But what is the spectrum of $A$ is not be purely discrete? If the spectrum of the self-adjoint operator $A$ has a continuous component, let $(E_\lambda)_{\lambda \in \mathbb{R}}$ be the projection-valued measure associated with $A$. Then the generalization of the spectral theorem allows us to write

$$A = \int \lambda dE_\lambda$$

and we have

$$\begin{aligned} \langle \psi, A\psi \rangle &= \int \lambda d\langle \psi, E_\lambda \psi \rangle \\ \langle \psi, \mathbf{1}_B(A)\psi \rangle &= \int \mathbf{1}_B(\lambda) d\langle \psi, E_\lambda \psi \rangle = \int_B d\langle \psi, E_\lambda \psi \rangle \end{aligned}$$

where $d\langle \psi, E_\lambda \psi \rangle$ is a Borel measure.

**Heisenberg's uncertainty principle.** Consider a quantum system described on a Hilbert space $\mathcal{H}$. States of the systems are associated to vectors $\psi \in \mathcal{H}$, normalized so that $\|\psi\| = 1$. Since observable quantities are given by expectations of the form $\langle \psi, A\psi \rangle$, for self-adjoint operators $A$, the vector $\psi$ is only defined up to a phase (ie. $\psi$ and $e^{i\theta}\psi$ describe the same state, if $\theta \in \mathbb{R}$ is a constant).
Taking into account that $\psi$ determines simultaneously the distribution of all observables of the system, it follows that these distributions cannot be independent of each other. An important consequence of this observation is Heisenberg's uncertainty principle.

**Theorem 2.1.1.** *Let $A, B$ be two self-adjoint operators acting on a Hilbert space $\mathcal{H}$ and let $\psi \in \mathcal{H}$ be a normalized (so that $\|\psi\| = 1$). We define the variance of $A$ in the state $\psi$ by*

$$\Delta A_\psi = \langle \psi, (A - \langle \psi, A\psi \rangle)^2 \psi \rangle = \langle \psi, A^2 \psi \rangle - \langle \psi, A\psi \rangle^2$$

*Then, we have*

$$\Delta A_\psi \Delta B_\psi \geq \frac{1}{4}|\langle \psi, [A,B]\psi\rangle|^2$$

*Proof.* Replacing $A$ and $B$ by $\widetilde{A} = A - \langle \psi, A\psi\rangle$ and $\widetilde{B} = B - \langle \psi, B\psi\rangle$, we can assume that $\langle \psi, A\psi\rangle = \langle \psi, B\psi\rangle = 0$. Then

$$\langle \psi, [A,B]\psi\rangle = \langle \psi, AB\psi\rangle - \langle \psi, BA\psi\rangle = 2i\text{Im } \langle \psi, AB\psi\rangle$$

This implies that

$$|\langle \psi, [A,B]\psi\rangle| \leq 2|\langle \psi, AB\psi\rangle| = 2|\langle A\psi, B\psi\rangle| \leq 2\|A\psi\|\|B\psi\| = 2\Delta A_\psi^{1/2}\Delta B_\psi^{1/2}$$

and therefore that

$$\Delta A_\psi \Delta B_\psi \geq \frac{1}{4}|\langle \psi, [A,B]\psi\rangle|^2$$

□

*Example.* Consider a particle moving on $\mathbb{R}$, take $A = x$ and $B = -i\hbar\partial_x$. Then $[A,B] = i\hbar$. It follows that

$$\Delta x_\psi \Delta p_\psi \geq \frac{\hbar^2}{4}$$

In other words, $x$ and $p$ cannot be measured simultaneously with arbitrary precision. If $\psi$ concentrates very much around a position $x_0$ (meaning that the variance $\Delta x_\psi$ is very small), then $\hat{\psi}$ is flat, meaning that the variance $\Delta p_\psi$ is large. Only commuting observables can be measured simultaneously.

**The Hamilton operator and the time evolution.** In every quantum system there is an observable that plays a particularly important role. The Hamilton operator, or the Hamiltonian, is a self-adjoint operator $H$ on the Hilbert space $\mathcal{H}$, corresponding to the energy of the system. Through the Schrödinger equation

$$i\partial_t \psi(t) = H\psi(t) \tag{2.3}$$

for $\psi(t) \in \mathcal{H}$, the Hamilton operator generates the time evolution of the quantum system. Notice that

$$\begin{aligned}\frac{d}{dt}\|\psi(t)\|^2 &= \frac{d}{dt}\langle \psi(t), \psi(t)\rangle \\ &= i\left[\langle i\partial(t)\psi(t), \psi(t)\rangle - \langle \psi(t), i\partial_t\psi(t)\rangle\right] \\ &= i\left[\langle H\psi(t), \psi(t)\rangle - \langle \psi(t), H\psi(t)\rangle\right] \\ &= 0\end{aligned}$$

since $H$ is self-adjoint. Hence, the Schrödinger equation defines a unitary evolution on $\mathcal{H}$, preserving the norm. Denoting by $e^{-iHt}$ the unitary group generated by $H$, we can write the solution of the Schrödinger equation (2.3) with initial data $\psi(0)$ as $\psi(t) = e^{-iHt}\psi(0)$.

Suppose that $\varphi \in \mathcal{H}$ is a normalized eigenvector of $H$, ie $H\varphi = E\varphi$. Then, the solution of the Schrödinger equation with initial data $\psi(0) = \varphi$ is simply given by $\psi(t) = e^{-iEt}\varphi$. This implies that

$\langle \psi(t), A\psi(t)\rangle = \langle \varphi, A\varphi\rangle$, independently of $t$. For this reason, eigenvectors of $H$ are referred to as stationary states.

Consider now a quantum particle in $\mathbb{R}^d$, described on the Hilbert space $L^2(\mathbb{R}^d)$. As explained above, the observables depending on the position are associated with multiplication operators, while the momentum is associated with the differential operator $p = -i\nabla$. Recalling the classical energy $\mathcal{H} = p^2/(2m) + V(x)$, we can guess that the Hamilton operator for this system takes the form

$$H = -\frac{\Delta}{2m} + V(x) \tag{2.4}$$

where $\Delta = \nabla \cdot \nabla$ is the Laplace operator on $H^2(\mathbb{R}^d)$. Operators of the form (2.4) are known as Schrödinger operators. Understanding their spectral properties is crucial to understand properties of the time-evolution they generate.

**Conservation laws.** Let $A$ be a self-adjoint operator on the Hilbert space $\mathcal{H}$. Let $\psi(t)$ denote the solution of the Schrödinger equation

$$i\partial_t \psi(t) = H\psi(t)$$

The variation of the expectation of the observable $A$ has the form

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

where $[A, H] = AH - HA$ is the commutator between the operators $A$ and $H$. This should be compared with the Poisson brakets in the classical setting; the commutator replaces here the Poisson brackets.

In particular, for an observable $A$ satisfying $[A, H] = 0$, the expectation $\langle \psi(t), A\psi(t)\rangle$ remains constant over time.

**The free Schrödinger Equation.** If there is no interaction and the quantum particle is moving freely, we talk about the free Schrödinger equation. In such case the Hamiltonian reads $H = -\Delta/2m$ on $H^2(\mathbb{R}^d)$ (this is the Hamilton operator of a free particle moving in $\mathbb{R}^d$), then $[H, -i\nabla] = 0$, ie. momentum is conserved. Similarly, the Hamilton operator $H = -\Delta/2m + V(|x|)$ acting on $H^2(\mathbb{R}^3)$, with a radial potential (ie. $V$ only depends on the $\|x\|$), then $[H, x \wedge -i\nabla] = 0$, ie. (each component of) the angular momentum operator $L = -ix \wedge \nabla$ is conserved. We will use this conservation law below, to compute the spectrum of the Hamilton operator describing the hydrogen atom.

*Example: the Stern-Gerlach experiment.* In quantum mechanics, elementary particles have an internal degree of freedom, known as spin. The spin is an angular momentum; it has three components, $\sigma_x$, $\sigma_y$, $\sigma_z$. Experimentally, the existence of a spin can be verified with a Stern-Gerlach experiment, using the fact that spins couple to magnetic fields. In the Stern-Gerlach experiment, neutral particles (in the original experiment in 1922, silver atoms) are sent through a non-constant magnetic field, which deflects them according to their spin. Particles are then detected on a screen. The outcome of the experiment was, at the beginning, surprising (it led to the Nobel Prize for Stern in 1943); the screen does not show a continuous distribution but, instead, it reveals discrete accumulation points, showing that the spin (more precisely, the component of the spin in the direction parallel to the applied magnetic field) is quantized. Particles are associated with a spin number $n \in \mathbb{N}/2$; each

spin component has then $2n+1$ possible values. In particular, for spin $1/2$ particles (like electrons, protons), each spin component has two possible values (spin up or spin down).
If we forget about all other degrees of freedom, we can describe the setting of the Stern-Gerlach experiment, restricting for simplicity our attention to spin $1/2$ particles, as a quantum system on $\mathbb{C}^2$. If the magnetic field in the Stern-Gerlach apparatus points in the $z$-direction, it is convenient to choose the vectors $(1,0),(0,1) \in \mathbb{C}^2$ to describe particles with the $z$-component of the spin pointing up and, respectively, down. In this representation of the system, the $z$-component of the spin is associated with the self-adjoint matrix

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.5}$$

The $x$- and the $y$-component of the spin are associated instead with the matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{2.6}$$

The matrices $\sigma_x, \sigma_y, \sigma_z$ are known as Pauli matrices. They satisfy the commutation relation

$$[\sigma_x, \sigma_y] = 2i\sigma_z \tag{2.7}$$

and its cyclic permutations. In particular, notice that spins in different directions do not commute. Notice that we did not try to justify the choice of the matrices (2.5), (2.6). In fact, as we will discuss later, relations between operators associated to different spin components (in particular the commutator relations (2.7)), are determined by the properties of the group of rotations $SO(3)$.
The Stern Gerlach experiment is a measurement of the z-component of the spin. If the initial state of the system is described by the vector $\psi = (\alpha, \beta) \in \mathbb{C}^2$, normalized so that $|\alpha|^2 + |\beta|^2 = 1$, the measurement of $\sigma_z$ will give the value $+1$ with probability $|\alpha|^2$ and the value $-1$ with probability $|\beta|^2$. In other words, after going through the Stern-Gerlach appartus, the particle will move up and hit the upper accumulation point on the screen with probability $|\alpha|^2$ and it will move down and hit the lower accumulation point on the screen with probability $|\beta|^2$. If the measurement of $\sigma_z$ gives the value $+1$, after going through the apparatus the particle is described by the vector $(1,0)$. In this case, if we let the particle go through a second Stern-Gerlach experiment, again with magnetic field pointing in the $z$ direction, the particle will show spin up with probability one. On the other hand, if the measurement of $\sigma_z$ gives the value $-1$, after going through the apparatus the particle is described by the vector $(0,1)$. In this case, a second measurement of $\sigma_z$ will give again the value $-1$ with probability one. It is also possible to insert, after the first Stern-Gerlach apparatus measuring the $z$-component of the spin, a Stern-Gerlach apparatus measuring, say, the $x$-component of the spin. Let us assume, for example, that the first measurement of $\sigma_z$ returns the value $+1$ and therefore that after the first measurement the system is described by the vector $(1,0)$. The expectation value of $\sigma_x$ is given by

$$\left\langle (1,0), \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} (1,0) \right\rangle = 0$$

Since $\sigma_x^2 = 1$, the variance of $\sigma_x$ is given by $\Delta\sigma_x = 1$. A different approach to reach the same conclusion consists in noticing that the matrix $\sigma_x$ has the two eigenvalues $\pm 1$ associated with the normalized eigenvectors $(1/\sqrt{2}, 1/\sqrt{2})$ and $(1/\sqrt{2}, -1/\sqrt{2})$. Since

$$(1,0) = \frac{1}{\sqrt{2}}(1/\sqrt{2}, 1/\sqrt{2}) + \frac{1}{\sqrt{2}}(1/\sqrt{2}, -1/\sqrt{2})$$

we conclude that the measurement of $\sigma_x$ gives the value $+1$ and the value $-1$ both with probability $1/2$ (this explains also why the expectation of $\sigma_x$ vanishes and its variance equals one). This result shows a well-known phenomenon in quantum systems. Non-commuting observables cannot be measured simultaneously. It is impossible to know the precise value of $\sigma_z$ and of $\sigma_x$ at the same time (mathematically, this means that two non-commuting self-adjoint operators cannot be diagonalized simultaneously).

**Density matrices and mixed states.** As explained above a quantum mechanical system is described on a Hilbert space $\mathcal{H}$. States of the system are associated with normalized vectors $\psi \in \mathcal{H}$. Observables are associated with self-adjoint operators $A$ acting on $\mathcal{H}$. The expectation value for the measurement of the observable $A$ in the state $\psi$ is then given by the inner product $\langle \psi, A\psi \rangle$. The same state can be described through the orthogonal projection onto $\psi$, denoted by

$$\gamma = |\psi\rangle\langle\psi|$$

The expectation of the observable $A$ is then given by

$$\langle \psi, A\psi \rangle = \mathrm{tr} A\gamma$$

In this case, describing the system through $\gamma$ is fully equivalent to the description given by $\psi$. Moreover, observe that the description through $\gamma$ shows that $e^{i\theta}\psi$ and $\psi$ describe the same state. The description through $\gamma$ has the advantage that it can be easily extended to mixed states.

**Definition 2.1.2.** *A density matrix over the Hilbert space $\mathcal{H}$ is a non-negative (in particular self-adjoint) trace class operator $\gamma$ on $\mathcal{H}$, with $tr\gamma = 1$. A trace class operator is a compact operator, with the property that the sequence $\{\lambda_j\}_j$ of its eigenvalues is summable, ie. $\sum_j |\lambda_j| < \infty$. The trace of a trace class operator $\gamma$ is defined by $tr\gamma = \sum_j \lambda_j$*

Given a density matrix $\gamma$ over $\mathcal{H}$, we can always decompose it as

$$\gamma = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$$

where $\{\psi_j\}_j$ is an orthonormal basis in $\mathcal{H}$ and where $\lambda_j \geq 0$ for all $j$, with $\sum_j \lambda_j = 1$. Such a density matrix describes the system, if it is in the state $\psi_j$ with probability $\lambda_j$. If the density matrix $\gamma$ is not an orthogonal projection, it is said to describe a mixed state (on the other hand, if $\gamma = |\psi\rangle\langle\psi|$ is an orthogonal projection, it is said to describe the pure state, which can be equivalently be described by the vector $\psi \in \mathcal{H}$).

There is an important consequence of being a pure or a mixed state, which is connected to the information we have on the quantum system. Consider pure states, given by linear combinations

of vectors in $\mathcal{H}$, and mixed states, given by a density matrix that is a (convex) linear combination of orthogonal projections. Suppose for example $\psi_1, \psi_2$ are two orthogonal normalized vectors in $\mathcal{H}$. Then

$$\psi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2) \tag{2.8}$$

is again a normalized vector in $\mathcal{H}$. The expectation of an observable $A$ in the pure state $\psi$ is given by

$$\langle \psi, A\psi \rangle = \frac{1}{2} \left[ \langle \psi_1, A\psi_1 \rangle + \langle \psi_2, A\psi_2 \rangle + \langle \psi_1, A\psi_2 \rangle + \langle \psi_2, A\psi_1 \rangle \right] \tag{2.9}$$

On the other hand, consider the mixed state, described by the density matrix

$$\gamma = \frac{1}{2} \left[ |\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| \right] \tag{2.10}$$

The expectation of $A$ in the mixed state with density matrix $\gamma$ is given by

$$\mathrm{tr} A\gamma = \frac{1}{2} \left[ \langle \psi_1, A\psi_1 \rangle + \langle \psi_2, A\psi_2 \rangle \right]$$

In contrast to (2.9), there are here no "interference" terms of the form $\langle \psi_1, A\psi_2 \rangle$, $\langle \psi_2, A\psi_1 \rangle$. We call (2.8) a coherent superposition of the quantum states $\psi_1, \psi_2$. On the other hand, (2.10) is called an incoherent superposition of quantum states.
Mixed states are needed, when there is no complete information about the system. For example, equilibrium states at positive temperature are mixed.

## 2.2 Many-Body Quantum Mechanics

**Bosonic and fermionic statistics.** A system of $N$ particles moving in the 3-dimensional space is described on the Hilbert space

$$\mathcal{H}_N = L^2(\mathbb{R}^{dN}, dx_1 \dots dx_N) = L^2(\mathbb{R}^3)^{\otimes N}$$

given by the tensor product of $N$ copies of the one-particle space $L^2(\mathbb{R}^3)$. Wave functions $\psi_N \in \mathcal{H}_N$ are normalized so that

$$\|\psi_N\|^2 = \int |\psi_N(x_1, \dots, x_N)|^2 \, dx_1 \dots dx_N = 1$$

Accordingly, $|\psi_N(x_1, \dots, x_N)|^2$ is the probability density for finding particle 1 close to $x_1$, particle 2 close to $x_2$, and so on.
When considering systems of $N$ indistinguishable particles, we need to restrict the Hilbert space to subspaces with appropriate statistics. Indistinguishability plays an important role in quantum mechanics, much more important than in classical mechanics. Classical particles follow trajectories and can be labeled. Quantum particles do not. Indistinguishability translates, in quantum system, into a restriction of the set of physical observables. Only observables that are invariant with respect to permutations of the $N$ particles can be measured.

Let us denote by $S_N$ the group of permutations $\pi$ of the set $\{1, 2, \dots, N\}$. We define a unitary representation of $S_N$ on the $N$-particle Hilbert space $L^2(\mathbb{R}^{3N})$ setting

$$(U_\pi \psi)(x_1, \dots, x_N) = \psi(x_{\pi 1}, \dots, x_{\pi N})$$

Physically meaningful observables of the $N$-particle system are self-adjoint operators $A$ on $L^2(\mathbb{R}^{3N})$ with the property $U_\pi^* A U_\pi = A$ (or, equivalently, $[A, U_\pi] = 0$) for all $\pi \in S_N$.
The existence of such unitary representation is justified by the Abelianization of the group of permutations. More precisely, there exists a homeomorphism $e^{i\theta(\cdot)} : S_N \to U(1)$, where $U(1)$ is the unit circle, that is a one-dimensional representation of the symmetric group. We can therefore consider the Abelianization of $S_N$ with the standard procedure[1] and construct the Abelian group $S_N/[S_N, S_N]$. Observe that in dimension $d \geq 3$ this is topologically justified (whereas for $d = 2$ there are infinitely many choices for $\theta$). The largest Abelian quotient is then made of two elements: the identity and the parity of the permutation. Since any one-dimensional representation must factor through the Abelianization, there are only two possibilities: for every $\pi \in S_N$, either $e^{i\theta(\pi)} = 1$ or $e^{i\theta(\pi)} = (-1)^{\mathrm{sgn}(\pi)}$, where $\mathrm{sgn}(\pi)$ is the sign of the permutation $\pi$. More precisely, if $\pi$ consists of an even number of transpositions, $\sigma_\pi = -1$ if $\pi$ consists of an odd number of transpositions). For each quantum particle, either completely symmetric or completely antisymmetric wave functions can be considered, not both at the same time. Particles described by wave functions that are symmetric w.r.t. permutations are called bosons. Particles described by antisymmetric wave function are called fermions. Systems of $N$ bosons moving in the three dimensional space are described on the Hilbert space

$$L^2_s(\mathbb{R}^{3N}) = L^2(\mathbb{R}^3)^{\otimes_s N} = \{\psi \in L^2(\mathbb{R}^{3N}) : \psi(x_{\pi 1}, \dots, x_{\pi N}) = \psi(x_1, \dots, x_N)\}$$

Systems of $N$ fermions on $\mathbb{R}^3$ are described, on the other hand, on the Hilbert space

$$L^2_a(\mathbb{R}^{3N}) = L^2(\mathbb{R}^3)^{\wedge N} = \{\psi \in L^2(\mathbb{R}^{3N}) : \psi(x_{\pi 1}, \dots, x_{\pi N}) = \sigma_\pi \psi(x_1, \dots, x_N)\}$$

The choice between bosonic and fermionic statistics is related with the internal degree of freedom of quantum particles, known as spin (already discussed in the Stern-Gerlach experiment). Particles with integer spin are bosons (they are described by wave functions that are symmetric w.r.t. permutations). Particles with half-integer spin are fermions (they must be described by wave functions that are antisymmetric w.r.t. permutations).

*Examples of bosonic wave function:* The simplest example of a bosonic wave function is the product of $N$ copies of the same one-particle normalized wave function $\varphi \in L^2(\mathbb{R}^3)$, ie

$$\psi_N(x_1, \dots, x_N) = \prod_{j=1}^{N} \varphi(x_j)$$

which is clearly normalized and symmetric w.r.t. permutations.

[1] By Abelianization of a group $G$ we refer to the existence of a homeomorphism $h : G \mapsto G'$ such that $G'$ is Abelian. Such homeomorphism can be constructed by considering the kernel given by the commutator subgroup $[G, G]$, which is the unique smallest normal subgroup of $G$ such that the quotient group $G' = G/[G, G]$ is Abelian.

More generally, if $\{\varphi_j\}_{j\in\mathbb{N}}$ is an orthonormal basis in $L^2(\mathbb{R}^3)$, we can describe the $N$-particle state with one particle in the state $\varphi_{i_1}$, one particle in the state $\varphi_{i_2}$, and so on, the symmetrized wave function

$$\psi_B(x_1,\dots,x_N)=\sqrt{\frac{1}{\ell_1!\ell_2!\dots\ell_k!N!}}\sum_{\pi\in S_N}\varphi_{i_1}(x_{\pi_1})\varphi_{i_2}(x_{\pi 2})\dots\varphi_{i_N}(x_{\pi N})$$

if the set $\{i_1,\dots,i_N\}$ contains $k$ different indices, appearing respectively $\ell_1,\dots\ell_k$ times, with $\ell_1+\ell_2+\dots+\ell_k=N$.
Similarly, we can construct fermionic wave functions. In this case, however, each one-particle state can be "occupied" by at most one-particle, otherwise the antisymmetrization is going to vanish (this is known as the Pauli principle). The fermionic state with one particle in the state $\varphi_{i_1}$, one particle in the state $\varphi_{i_2}$, and so on (with all different indices $i_1,\dots,i_N$) , can be described by the wave function

$$\psi_F(x_1,\dots,x_N)=\frac{1}{\sqrt{N!}}\sum_{\pi\in S_N}\sigma_\pi\varphi_{i_1}(x_{\pi 1})\dots\varphi_{i_N}(x_{\pi N})$$

The wave function $\psi_F$ can be written as

$$\psi_F(x_1,\dots,x_N)=\frac{1}{\sqrt{N!}}\det\,(\varphi_{i_j}(x_k))_{1\le j,k\le N}$$

Such wave functions are known as Slater determinants.

**Reduced density matrices.** The density matrix of a normalized $N$-particle wave function $\psi_N\in L^2(\mathbb{R}^{3N})$, with either bosonic or fermionic statistics, is defined as $\gamma_N=|\psi_N\rangle\langle\psi_N|$, ie. $\gamma_N$ is the orthogonal projection onto $\psi_N$. More generally, mixed states of an $N$-particle system are described by non-negative trace class operators $\gamma_N$ with $\mathrm{tr}\gamma_N=1$.
For a density matrix $\gamma_N$, we denote by $\gamma_N(x_1,\dots,x_N;y_1,\dots,y_N)$ the integral kernel of $\gamma_N$. This is defined so that

$$(\gamma_N\xi_N)(x_1,\dots,x_N)=\int\gamma_N(x_1,\dots,x_N;y_1,\dots,y_N)\xi_N(y_1,\dots,y_N)$$

Every trace class operator can be associated with an integral kernel (since every trace class operator is Hilbert Schmidt, the integral kernel is in fact a $L^2(\mathbb{R}^{3N}\times\mathbb{R}^{3N})$-function).
Using the integral kernel of $\gamma_N$, we can define its reduced density matrices. For $1\le k\le N$, we define the $k$-particle reduced density matrix associated with $\gamma_N$ (and therefore with $\psi_N$) by

$$\gamma^{(k)}=\frac{N!}{(N-k)!}\mathrm{tr}_{k+1,k+2,\dots,N}\gamma_N$$

where $\mathrm{tr}_{k+1,\dots,N}\gamma_N$ denotes the partial trace of $\gamma_N$ over the last $(N-k)$ particles. Taking the partial trace means integrating out the degrees of freedom associated with the last $(N-k)$ particles. In other words, $\gamma_N^{(k)}$ is defined through its integral kernel

$$\begin{aligned}&\gamma_N^{(k)}(x_1,\dots,x_k;y_1,\dots,y_k)\\&\quad=\frac{N!}{(N-k)!}\int\gamma_N(x_1,\dots x_k,x_{k+1},\dots,x_N;y_1,\dots y_k,x_{k+1},\dots,x_N)dx_{k+1}\dots dx_N\end{aligned}$$

By definition, it is easy to check that $\gamma_N^{(k)}$ is a non-negative operator, for all $1 \leq k \leq N$. In fact, for an arbitrary $\varphi \in L^2(\mathbb{R}^{3k})$ we have

$$\begin{aligned}\langle \varphi, \gamma^{(k)} \varphi \rangle &= \int dx_1 \dots dx_k \, dy_1 \dots dy_k \bar{\varphi}(x_1, \dots, x_k) \gamma_N^{(k)}(x_1, \dots, x_k; y_1, \dots, y_k) \varphi(y_1, \dots, y_k) \\ &= \int dx_{k+1} \dots dx_N \left| \int dx_1 \dots dx_k \, \bar{\varphi}(x_1, \dots, x_k) \psi_N(x_1, \dots, x_k, x_{k+1}, \dots, x_N) \right|^2 \geq 0\end{aligned}$$

Moreover,

$$\mathrm{tr} \gamma_N^{(k)} = \frac{N!}{(N-k)!} \int dx_1 \dots dx_k \gamma_N^{(k)}(x_1, \dots, x_k; x_1, \dots, x_k) = \frac{N!}{(N-k)!}$$

Reduced density matrices are useful, because they allow us to compute the expectation of observables that depend only on a fixed number $k$ of particles. Let $\mathcal{O}^{(k)}$ be an operator on the $k$-particle space $L^2(\mathbb{R}^{3k})$. Then $\mathcal{O}^{(k)} \otimes 1^{(N-k)}$ is an operator on $L^2(\mathbb{R}^{3N})$, acting as $\mathcal{O}^{(k)}$ on the first $k$ particles and as the identity on the other $(N-k)$ particles. A simple computation shows that

$$\langle \psi_N, (\mathcal{O}^{(k)} \otimes 1^{(N-k)}) \psi_N \rangle = \frac{(N-k)!}{N!} \mathrm{tr} \, \mathcal{O}^{(k)} \gamma_N^{(k)}$$

where, on the r.h.s., tr denotes the trace over $L^2(\mathbb{R}^{3k})$. Interesting $k$-particle observables in $N$-body systems must be invariant w.r.t. permutations of the $N$ particles and are therefore given by sums over all possible choices of the $k$ indices, over which $\mathcal{O}^{(k)}$ must act non-trivially. Using the permutation invariance of $\psi_N$, their expectation is given by

$$\sum_{1 \leq i_1 < i_2 < \dots < i_k \leq N} \langle \psi_N, \mathcal{O}^{(k)}_{i_1, \dots, i_k} \psi_N \rangle = \sum_{1 \leq i_1 < i_2 < \dots < i_k \leq N} \frac{(N-k)!}{N!} \mathrm{tr} \, \mathcal{O}^{(k)} \gamma_N^{(k)} = \frac{1}{k!} \mathrm{tr} \, \mathcal{O}^{(k)} \gamma_N^{(k)}$$

For example, the kinetic energy of an $N$-body system is the one-particle operator $\sum_{j=1}^N -\Delta_{x_j}$. Its expectation in the state $\psi_N$ can be computed through the one-particle reduced density $\gamma_N^{(1)}$:

$$\langle \psi_N, \sum_{j=1}^N -\Delta_{x_j} \psi_N \rangle = \mathrm{tr}(-\Delta) \gamma_N^{(1)}$$

A two-body interaction has the form $\sum_{i<j}^N V(x_i - x_j)$. To compute its expectation we need its 2-particle reduced density:

$$\langle \psi_N, \sum_{i<j}^N V(x_i - x_j) \psi_N \rangle = \frac{1}{2} \mathrm{tr} V(x_1 - x_2) \gamma_N^{(2)}$$

Let us compute a couple of reduced density matrices, for simple example of $N$-particle states. In the bosonic setting, the simplest class of $N$-particle states are factorized wave functions of the form $\psi_N(x_1, \dots, x_N) = \prod_{j=1}^N \varphi(x_j)$. In this case, it is very easy to compute reduced density matrices. We find

$$\gamma_N^{(k)} = \frac{N!}{(N-k)!} |\varphi\rangle\langle\varphi|^{\otimes k}$$

where $|\varphi\rangle\langle\varphi|$ is the orthogonal projection onto $\varphi$.
In the fermionic setting, the simplest class of $N$-particle states are Slater determinant, having the form

$$\psi_N(x_1,\dots,x_N) = \frac{1}{\sqrt{N!}}\det\ (\varphi_i(x_j))_{1\leq i,j\leq N}$$

where $\{\varphi_j\}_{j=1}^N$ is an orthonormal system on $L^2(\mathbb{R}^3)$. The one-particle reduced density matrix associated with $\psi_N$ has the integral kernel

$$\begin{aligned}\gamma_N^{(1)}(x;x') &= \frac{N}{N!}\sum_{\pi,\pi'\in S_N}\sigma_\pi\sigma_{\pi'}\varphi_{\pi 1}(x)\varphi_{\pi' 1}(x')\int dx_2\dots dx_N\ \prod_{j=2}^N \varphi_{\pi j}(x_j)\varphi_{\pi' j}(x_j)\\ &= \frac{1}{(N-1)!}\sum_\pi \varphi_{\pi 1}(x)\varphi_{\pi 1}(x') = \sum_{j=1}^N \varphi_j(x)\varphi_j(x')\end{aligned}$$

Hence $\gamma_N^{(1)} = \sum_{j=1}^N |\varphi_j\rangle\langle\varphi_j|$ is the orthogonal projection onto the $N$-dimensional subspace of $L^2(\mathbb{R}^3)$, spanned by $\varphi_1,\dots,\varphi_N$. Similarly, one can compute higher order reduced density matrices of the Slater determinant $\psi_N$. It turns out, they satisfy Wick's theorem, stating that

$$\gamma_N^{(k)}(x_1,\dots x_k;x_1',\dots,x_k') = \sum_{\pi\in S_k}\sigma_\pi\prod_{j=1}^k \gamma_N^{(1)}(x_j;x'_{\pi j})$$

In particular, the 2-particle reduced density is given by

$$\gamma_N^{(2)}(x_1,x_2;x_1',x_2') = \gamma_N^{(1)}(x_1;x_1')\gamma_N^{(1)}(x_2;x_2') - \gamma_N^{(1)}(x_1;x_2')\gamma_N^{(1)}(x_2;x_1')$$

Typical $N$-particle Hamilton operators have the form

$$H_N = \sum_{j=1}^N \big[-\Delta_{x_j} + V_{\rm ext}(x_j)\big] + \sum_{i<j} V(x_i-x_j)$$

The first term is a one-particle operator, it describes the kinetic energy of the particles and their interaction with external fields. The second term is a two-body operator, describing the interaction among the particles. The energy of the $N$-particle system in a state $\psi_N$ can be expressed in terms of the reduced density matrix $\gamma_N^{(2)}$ associated with $\psi_N$. We find

$$\langle\psi_N, H_N\psi_N\rangle = \mathrm{tr}\,\big[-\Delta + V_{\rm ext}\big]\gamma_N^{(1)} + \frac{1}{2}\mathrm{tr}\,V(x_1-x_2)\gamma_N^{(2)} \tag{2.11}$$

This identity suggests that a possible approach to compute the ground state energy of an $N$-particle system, ie. the infimum of $\langle\psi_N, H_N\psi_N\rangle$ over all normalized wave functions $\psi_N\in L^2(\mathbb{R}^{3N})$ with the appropriate statistics, consists in minimizing the r.h.s. of (2.11) over all possible choices of $\gamma_N^{(2)}$ (the one-particle density matrix $\gamma_N^{(1)}$ can be computed from $\gamma_N^{(2)}$, taking the partial trace over one of the two particles).
While in the bosonic case every non-negative trace class operator $\gamma^{(1)}$ over $L^2(\mathbb{R}^3)$ with $\mathrm{tr}\gamma^{(1)} = N$ is admissible, in the fermionic case admissibility requires the additional condition $\gamma^{(1)}\leq 1$, expressing the Pauli principle.

**Theorem 2.2.1.** *Let $\gamma^{(1)}$ be a self-adjoint, non-negative, trace-class operator on $L^2(\mathbb{R}^3)$, with $tr\gamma^{(1)} = N$, for some $N \in \mathbb{N}$. Then there exists a fermionic density matrix $\gamma$ over $L^2(\mathbb{R}^{3N})$ with $\gamma^{(1)} = N tr\gamma$ if and only if $\gamma^{(1)} \leq 1$.*

*Remarks:* 1) a density matrix $\gamma$ over $L^2(\mathbb{R}^{3N})$ is called fermionic if

$$\gamma(x_{\pi 1}, \dots x_{\pi N}; x'_{\pi' 1}, \dots, x'_{\pi' N}) = \sigma_\pi \sigma_{\pi'} \gamma(x_1, \dots, x_N; x'_1, \dots, x'_N)$$

for all permutations $\pi, \pi' \in S_N$; 2) in general $\gamma$ cannot be chosen as a pure state.

*Proof.* First, we assume $0 \leq \gamma^{(1)} \leq 1$ and we show the existence of $\gamma$ on $L^2(\mathbb{R}^{3N})$ with the desired properties. Suppose that

$$\gamma^{(1)} = \sum_j \lambda_j |\varphi_j\rangle\langle\varphi_j|$$

where $\varphi_j$ is an orthonormal system in $L^2(\mathbb{R}^3)$. We assume here that the eigenvalues $\lambda_j$ are ordered, ie.

$$1 \geq \lambda_1 \geq \lambda_2 \geq \dots$$

If $\lambda_{N+1} = 0$, the condition $\sum_j \lambda_j = N$ implies that $\lambda_j = 1$ for all $j = 1, \dots, N$, and therefore that $\gamma^{(1)} = \sum_{j=1}^N |\varphi_j\rangle\langle\varphi_j|$. In this case, the statement follows taking

$$\psi(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \sigma_\pi \varphi_{\pi 1}(x_1) \dots \varphi_{\pi N}(x_N)$$

as a Slater determinant in $L^2(\mathbb{R}^{3N})$ and setting $\gamma = |\psi\rangle\langle\psi|$.

Hence, we can assume that $\lambda_{N+1} > 0$. Because of the ordering of the eigenvalues, we have

$$N \geq \sum_{j=1}^{N+1} \lambda_j \geq (N+1)\lambda_{N+1} \tag{2.12}$$

which implies that $\lambda_{N+1} \leq N/(N+1) < 1$. Hence, defining

$$\varepsilon = \min\{\lambda_N, 1 - \lambda_{N+1}\}$$

we certainly have $0 < \varepsilon < 1$. Using the notation

$$\chi_{[1,N]}(j) = \begin{cases} 0 & \text{if } j > N \\ 1 & \text{if } 1 \leq j \leq N \end{cases}$$

we write

$$\lambda_j = \varepsilon \chi_{[1,N]}(j) + (1 - \varepsilon) f_j$$

with

$$f_j = \frac{1}{1-\varepsilon} \big[\lambda_j - \varepsilon \chi_{[1,N]}(j)\big]$$

We observe that, for $1 \leq j \leq N$, we have

$$f_j = \frac{\lambda_j - \varepsilon}{1 - \varepsilon}$$

and therefore $0 \leq f_j \leq 1$ (because $\lambda_j \geq \lambda_N \geq \varepsilon$ and $\lambda_j \leq 1$, for all $1 \leq j \leq N$). On the other hand, for $j > N$, we find

$$f_j = \frac{\lambda_j}{1 - \varepsilon}$$

and therefore again $0 \leq f_j \leq 1$, because $\lambda_j \leq \lambda_{N+1} \leq 1 - \varepsilon$ (from the choice $\varepsilon < 1 - \lambda_{N+1}$). Hence, we find $0 \leq f_j \leq 1$ for all $j$ and

$$\sum_j f_j = \frac{1}{1 - \varepsilon}(N - \varepsilon N) = 1$$

In other words, the coefficients $f_j$ satisfy the same conditions as the original coefficients $\lambda_j$.

After reshuffling the terms so that the coefficients $f_j$ are decreasing, we can repeat the procedure. After $M$ iteration, we arrive at

$$\lambda_j = \sum_{k=1}^{M} c_k \chi_k(j) + R_j^M \tag{2.13}$$

where

$$c_k = \varepsilon_k \prod_{j=1}^{k-1}(1 - \varepsilon_j),$$

$0 < \varepsilon_j < 1$ is the $\varepsilon$-coefficient used in the $j$-th iteration, $\chi_k$ is the characteristic function of a subset of $\mathbb{N}$ containing exactly $N$ points and

$$R_j^M = (1 - \varepsilon_1)(1 - \varepsilon_2) \dots (1 - \varepsilon_M) f_j^{(M)}$$

with $0 \leq f_j^{(M)} \leq 1$ for all $j$ and $\sum_j f_j^{(M)} = N$. Remark that

$$\prod_{k=1}^{M}(1 - \varepsilon_k) = 1 - \sum_{k=1}^{M} c_k \tag{2.14}$$

and therefore

$$R_j^M = f_j^{(M)}(1 - \sum_{k=1}^{M} c_k) \tag{2.15}$$

The identity (2.14) implies, in particular, that $\sum_{k=1}^{M} c_k \leq 1$, uniformly in $M$.

Now, we claim that, as $M \to \infty$,

$$\sum_{k=1}^{M} c_k \to 1. \tag{2.16}$$

By (2.15) (recalling that $0 \leq f_j^{(M)} \leq 1$), this would also imply that $R_j^M \to 0$ and therefore

$$\lambda_j = \sum_{k=1}^{\infty} c_k \chi_k(j)$$

which means that

$$\gamma^{(1)} = \sum_j \lambda_j |\varphi_j\rangle\langle\varphi_j| = \sum_{k=1}^{\infty} c_k \Big[ \sum_j \chi_k(j) |\varphi_j\rangle\langle\varphi_j| \Big]$$

Hence, $\gamma^{(1)}$ would be a convex (since $0 \leq c_k \leq 1$ for all $k \in \mathbb{N}$ and $\sum_{k=1}^{\infty} c_k = 1$) combination of projections onto $N$-dimensional subspaces of $L^2(\mathbb{R}^3)$. Introducing the notation $\psi_k \in L^2_a(\mathbb{R}^{3N})$ for the Slater determinant defined by the one-particle wave functions $\varphi_j$, for all $j$ with $\chi_k(j) = 1$ (for every $k \in \mathbb{N}$, there are exactly $N$ such labels $j$), we could conclude that

$$N \mathrm{tr}_{2,\ldots,N} |\psi_k\rangle\langle\psi_k| = \sum_j \chi_k(j) |\varphi_j\rangle\langle\varphi_j|$$

Defining the density matrix

$$\gamma = \sum_{k=1}^{\infty} c_k |\psi_k\rangle\langle\psi_k|$$

on $L^2_a(\mathbb{R}^{3N})$, we would obtain therefore that $N \mathrm{tr}_{2,\ldots,N} \gamma = \gamma^{(1)}$, as desired.

It remains to show the claim (2.16). Since $\sum_{k=1}^{M} c_k \leq 1$, uniformly in $M$, the limit $\lim_{M\to\infty} \sum_{k=1}^{M} c_k = d$ exists and satisfies $d \leq 1$. We proceed by contradiction and assume $d < 1$. From (2.13), also $\lim_{M\to\infty} R_j^M = R_j$ exists, for all $j$. By (2.15), it satisfies $0 \leq R_j \leq (1-d)$ and, by monotone convergence, $\sum_j R_j = \lim_{M\to\infty} \sum_j R_j^M = N(1-d)$, ie.

$$0 \leq \frac{R_j}{1-d} \leq 1 \quad \text{for all } j \text{ and} \quad \sum_j \frac{R_j}{1-d} = N \tag{2.17}$$

Let us write $f_j^{(M)} = R_j^M / (1 - \sum_{k=1}^{M} c_k)$. Then $f_j^{(M)} \to R_j/(1-d)$, as $M \to \infty$. We rearrange the coefficients $f_j^{(M)}$ so that the are monotonically decreasing. We call the resulting coefficients $\widetilde{f}_j^{(M)}$. Arguing as in (2.12), we find $1 - \widetilde{f}_{N+1}^{(M)} \geq 1/(N+1) > 0$, uniformly in $M$. On the other hand, $\widetilde{f}_N^{(M)}$ converges, as $M \to \infty$, to the $N$-th largest value in the sequence $R_j/(1-d)$. From (2.17), we know that this limit is strictly positive (because otherwise the sum of these coefficients could not reach $N$). Since $\varepsilon_{M+1} = \min(\widetilde{f}_N^{(M)}, 1 - \widetilde{f}_{N+1}^{(M)})$, it follows that $\varepsilon_M$ does not converge to 0. From (2.14), we conclude that $\sum_{k=1}^{M} c_k \to 1$, in contradiction to the assumption $d < 1$ (the limit of $\prod_{k=1}^{M} (1 - \varepsilon_k)$ is 0, unless the sequence $\varepsilon_k$ is summable).

Next, suppose that $\gamma^{(1)} = N \mathrm{tr}_{2,\ldots,N} \gamma$ for a fermionic density matrix $\gamma$ on $L^2(\mathbb{R}^{3N})$. We claim that $\gamma^{(1)} \leq 1$. It is enough to show the statement for pure states, ie if $\gamma = |\psi\rangle\langle\psi|$ for a normalized

$\psi \in L^2_a(\mathbb{R}^{3N})$. The general case follows by linearity. To this end, it is convenient to introduce creation and annihilation operators. For $\phi \in L^2(\mathbb{R}^3)$, we define $a_{N,\phi} : L^2_a(\mathbb{R}^{3N}) \to L^2_a(\mathbb{R}^{3(N-1)})$ setting

$$(a_{N,\phi}\psi)(x_1, \ldots, x_{N-1}) = \sqrt{N} \int dx \bar{\phi}(x)\psi(x, x_1, \ldots, x_{N-1})$$

We also define the creation operator $a^*_{N,\phi} : L^2_a(\mathbb{R}^{3(N-1)} \to L^2_a(\mathbb{R}^{3N})$, setting

$$(a^*_{N,\phi}\psi)(x_1, \ldots, x_N) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} (-1)^{N-j} \phi(x_j)\psi(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_N)$$

It is easy to check (as suggested by the notation, that $a^*_{N,\phi}$ is the adjoint of $a_{N,\phi}$, ie. that

$$\langle \psi_1, a_{N,\phi}\psi_2 \rangle = \langle a^*_{N,\phi}\psi_1, \psi_2 \rangle$$

Another important property of creation and annihilation operators is the identity:

$$a_{N+1,\phi}a^*_{N+1,\phi} + a^*_{N,\phi}a_{N,\phi} = \|\phi\|^2$$

Therefore, we obtain

$$\begin{aligned} \langle \phi, \gamma^{(1)}\phi \rangle &= \langle a_{N,\phi}\psi, a_{N,\phi}\psi \rangle = \langle \psi, a^*_{N,\phi}a_{N,\phi}\psi \rangle \\ &= -\langle \psi, a_{N+1,\phi}a^*_{N+1,\phi}\psi \rangle + \|\varphi\|^2 = -\|a^*_{N+1,\phi}\psi\|^2 + \|\varphi\|^2\|\psi\|^2 \leq \|\varphi\|^2 \end{aligned}$$

which proves that $\gamma^{(1)} \leq 1$. □

# 3 Stability of Matter

The core of this section is to introduce the Hamiltonian describing large atoms and molecules and study the properties leading to the proof of stability of matter.
The simplest class of many-body Hamilton operators consists of sums of one-body operators, having the form

$$H^{\text{free}}_N = \sum_{j=1}^{N} 1 \otimes \cdots \otimes h \otimes \cdots \otimes 1 \tag{3.18}$$

for a self-adjoint $h$ on the one-particle $L^2(\mathbb{R}^3)$. For example, the one-particle Hamilton operator may have the form $h = -\Delta + V_{\text{ext}}$. The time-evolution generated by (3.18) factorize, ie.

$$e^{-iH^{\text{free}}_N t} = e^{-iht} \otimes e^{-iht} \otimes \cdots \otimes e^{-iht}$$

In other words, the evolution of factorized initial data remains factorized and is determined by the one-particle Hamilton operator $h$. Similarly, eigenvectors of the non-interacting Hamilton operator $H^{\text{free}}_N$ are given by products of the eigenvectors of $h$. More precisely, for bosonic systems, $H^{\text{free}}_N$ acts on permutation symmetric functions, and its eigenvectors are symmetrized products of eigenvectors

of $h$. For fermionic systems, on the other hand, eigenvectors of $H_N^{\text{free}}$ are given by anti-symmetrized products of eigenvectors of $h$. Eigenvalues of $H_N^{\text{free}}$ are therefore given by sums of eigenvalues of $h$. For fermionic systems, because of Pauli's principle, only sums of eigenvalues that are associated with different eigenvectors are allowed. In particular, if $e_1 < e_2 \leq e_3 \leq \dots$ are the eigenvalues of $h$ (assuming the lowest eigenvalue to be simple), associated with the eigenvectors $\varphi_1, \varphi_2, \varphi_3, \dots$, the ground state energy of $H_N^{\text{free}}$ is given by $Ne_1$ in the bosonic case (corresponding to the eigenvector $\varphi_1^{\otimes N}$) and by $e_1 + e_2 + \dots + e_N$ in the fermionic case (corresponding with the Slater determinant $\det(\varphi_i(x_j))_{1\leq i,j\leq N}$). In particular, this implies that fermionic systems typically have a larger energy than bosonic systems, in the limit of large $N$.

We will now focus on a system of $N$ electrons and $M$ static nuclei, fixed at positions $R_1, \dots, R_M$ and with charges $Z_1, \dots, Z_M$ ($M = 1$ corresponds to an atom, $M > 1$ to a molecule). For $N, M \in \mathbb{N}$, $\mathbf{R} = (R_1, \dots, R_M) \in \mathbb{R}^{3M}$ and $\mathbf{Z} = (Z_1, \dots, Z_M) \in \mathbb{R}_+^M$ (physically, nuclei have integer charge, but the systems we are going to define make sense, mathematically, for arbitrary positive charges $Z_j$), we define the Hamilton operator

$$H_{N,M}(\mathbf{R}, \mathbf{Z}) = \sum_{j=1}^{N} \left[ -\Delta_{x_j} - \sum_{i=1}^{M} \frac{Z_i}{|R_i - x_j|} \right] + \sum_{i<j}^{N} \frac{1}{|x_i - x_j|} + \sum_{i<j}^{M} \frac{Z_i Z_j}{|R_i - R_j|} \tag{3.19}$$

We write $H_{N,M}(\mathbf{R}, \mathbf{Z}) = -\sum_{j=1}^{N} \Delta_{x_j} + V(\mathbf{R}, \mathbf{Z}, \mathbf{x})$, with the total potential energy operator

$$V(\mathbf{R}, \mathbf{Z}, \mathbf{x}) = \sum_{i<j}^{N} \frac{1}{|x_i - x_j|} + \sum_{i<j}^{M} \frac{Z_i Z_j}{|R_i - R_j|} - \sum_{j=1}^{N} \sum_{i=1}^{M} \frac{Z_i}{|R_i - x_j|}$$

Observing that

$$V(\mathbf{R}, \mathbf{Z}, \mathbf{x}) \geq -\sum_{j=1}^{N} \sum_{i=1}^{M} \frac{Z_i}{|R_i - x_j|} \tag{3.20}$$

and therefore that

$$H_{N,M}(\mathbf{R}, \mathbf{Z}) \geq \sum_{j=1}^{N} \sum_{i=1}^{M} \left[ \frac{-\Delta_{x_j}}{M} - \frac{Z_i}{|x_j - R_i|} \right]$$

we conclude, using the stability of the hydrogen atom, that

$$\inf_{\psi_N \in L^2(\mathbb{R}^3)^{\otimes N} : \|\psi_N\| = 1} \langle \psi_N, H_{N,M}(\mathbf{R}, \mathbf{Z}) \psi \rangle \geq -NM \sum_{i=1}^{M} Z_i^2 > -\infty \tag{3.21}$$

for every choice of $(\mathbf{R}, \mathbf{Z})$. Eq. (3.21) establishes stability of the first kind, which is essentially equivalent to the stability of the one-particle system (of the hydrogen atom, in this case).

From a physics viewpoint however such stability is not satisfactory. Indeed, if we consider the energy per particle by dividing both sides of the inequality by (N+M), which is the size of the particle system, we obtain a lower bound that grows with the number of particles. This observation leads to a new definition of stability, known as stability of the second kind, stating that the ground state

energy of a system with $N$ electrons and $M$ nuclei grows (in absolute value) at most linearly in the total number of particles $(N + M)$.

Compared with stability of the first kind, stability of the second kind is more difficult to prove and relies on one important physical property of matter: the Pauli principle, i.e. on the fact that electrons are fermions and must therefore be described by antisymmetric wave functions (stability of the first kind, on the other hand, holds independently of the statistics).

The next theorem establishes stability of the second kind for systems of electrons and nuclei described by the Hamilton operator (3.19). The goal of the rest of this section consists in proving this theorem.

**Theorem 3.0.1** (Stability of the second kind)**.** *Let*

$$E_{N,M}(\mathbf{R}, \mathbf{Z}) = \inf_{\psi \in L^2_a(\mathbb{R}^{3N}), \|\psi\|_2 = 1} \langle \psi_N, H_{N,M}(\mathbf{R}, \mathbf{Z}) \psi_N \rangle \,. \tag{3.22}$$

*denote the ground state energy of the Hamilton operator (3.19). Then we have*

$$E_{N,M}(\mathbf{Z}) = \inf\{E_{N,M}(\mathbf{R}, \mathbf{Z}) : \mathbf{R} = (R_1, \ldots, R_M) \in \mathbb{R}^{3M}\} \geq -C(Z)(N + M) \tag{3.23}$$

*where* $Z = \max(Z_1, \ldots, Z_M)$.

*Remark:* in the definition (3.19) of the Hamilton operator $H_{N,M}(\mathbf{R}, \mathbf{Z})$ we included the term $\sum_{i<j}^{M} Z_i Z_j / |R_i - R_j|$, describing the interaction among nuclei. Since nuclei are kept fixed in this model, this term is a constant. For stability of the first kind, it does not play any role (in fact, we estimated it by zero, in (3.20). For stability of the second kind, on the other hand, it plays a crucial role. Removing it, the infimum of the energy would be attained taking $R_1 = \cdots = R_M = 0$, which leads to the operator

$$H_{N,M}(\mathbf{R} = (0, \ldots, 0), \mathbf{Z}) = \sum_{j=1}^{N} \left[ -\Delta_{x_j} - \frac{(\sum_{i=1}^{M} Z_i)}{|x_j|} \right] + \sum_{i<j}^{N} \frac{1}{|x_i - x_j|} \tag{3.24}$$

Ignoring the interaction among the electrons, the ground state of (3.24) is of the order $-N(\sum_{i=1}^{M} Z_i)^2 \simeq -NM^2$. Since the effect of the interaction among the electrons can be bounded unformly in $M$, this would contradict stability of the second kind.

An important property of the ground state energy (3.22) is its monotonicity in the nuclear charges, to be understood in the sense of following proposition.

**Proposition 3.0.2.** *Assume* $Z_j \leq Z$ *for all* $j = 1, \ldots, M$ *(in other words,* $Z$ *is the maximal charge of the* $M$ *nuclei). Then*

$$E_{N,M}(\mathbf{R}, \mathbf{Z}) \geq \min_{M' \leq M} \min_{i_1 < i_2 < \cdots < i_{M'}} E_{N,M'}((R_{i_1}, \ldots, R_{i_{M'}}), (Z, \ldots, Z))$$

*Remark:* In other words, a lower bound for $E_{N,M}(\mathbf{R}, \mathbf{Z})$ can be obtained by replacing each nuclear charge $Z_k$ either by zero (which is equivalent to removing the nucleus) or by the common upper bound $Z$ (the maximal charge), and by taking the minimum over all such nuclear configurations.

*Proof.* Exercise. □

Another interesting observation concerns the role played by the restriction to permutation symmetric states. There is an important difference here between fermionic and bosonic systems. It turns out that the restriction on bosonic states has no effect in the search for minimizers (we will see later that the restriction on fermionic state, on the other hand, has important consequences for the minimizers; in fact stability of the second kind, as stated in (3.23), only holds true because of this restriction).

**Proposition 3.0.3.** *Let $\mathcal{E}(\psi)$ a quadratic form on $L^2(\mathbb{R}^{3N})$, with*

*i) $\mathcal{E}(\psi) \geq C\|\psi\|^2$ for a constant $C > -\infty$.*

*ii) $\mathcal{E}(|\psi|) \leq \mathcal{E}(\psi)$ for all $\psi \in L^2(\mathbb{R}^{3N})$.*

*iii) $\mathcal{E}(\psi_\pi) = \mathcal{E}(\psi)$ for all permutation $\pi \in S_N$, where $\psi_\pi(x_1, \ldots, x_N) = \psi(x_{\pi 1}, \ldots, x_{\pi N})$.*

*Then we have*

$$E_0 = \inf\{\mathcal{E}(\psi) : \|\psi\|_2 = 1\} = \inf\{\mathcal{E}(\psi) : \|\psi\|_2 = 1 \text{ and } \psi_\pi = \psi \text{ for all } \pi \in S_N\}$$

*Proof.* From a) we have $E_0 > -\infty$. From b), we have

$$\inf\{\mathcal{E}(\psi) : \|\psi\|_2 = 1\} = \inf\{\mathcal{E}(\psi) : \|\psi\|_2 = 1 \text{and } \psi = |\psi|\}$$

Since $|\psi|$ is permutation symmetric if $\psi$ is, we also obtain

$$\begin{aligned}\inf\{\mathcal{E}(\psi) : \|\psi\|_2 = 1 \text{ and } \psi_\pi = \psi \text{ for all } \pi \in S_N\}& \\ = \inf\{\mathcal{E}(\psi) : \|\psi\|_2 = 1, \psi = |\psi| \text{ and } \psi_\pi = \psi \text{ for all } \pi \in S_N\}&\end{aligned}$$

Suppose now that $\psi \geq 0$ is an unrestricted minimizer in $L^2(\mathbb{R}^{3N})$, ie. $\mathcal{E}(\psi) = E_0$ and $\|\psi\|_2 = 1$. Then we can decompose $\psi = \psi_s + \psi_r$, with

$$\psi_s = \frac{1}{N!} \sum_{\pi \in S_N} \psi_\pi$$

the symmetrization of $\psi$ ($\psi_r$ is defined as the reminder, ie. $\psi_r = \psi - \psi_s$). Observe that (since $\langle \psi_\pi, \psi_\sigma \rangle \geq 0$ for all $\pi, \sigma \in S_N$) $\|\psi_s\|^2 > 0$ (exercise), which implies that $\psi_s \neq 0$. Moreover, we have

$$\mathcal{E}(\psi) = \mathcal{E}(\psi_s) + \mathcal{E}(\psi_r) \tag{3.25}$$

To show (3.25), we define the sesquilinear form $Q : L^2(\mathbb{R}^{3N}) \times L^2(\mathbb{R}^{3N}) \to \mathbb{C}$ associated with $\mathcal{E}$, defined by

$$Q(\varphi, \psi) = \frac{1}{4i} \left[\mathcal{E}(\varphi + i\psi) - \mathcal{E}(\varphi - i\psi)\right] + \frac{1}{4} \left[\mathcal{E}(\varphi + \psi) - \mathcal{E}(\varphi - \psi)\right]$$

so that $\mathcal{E}(\psi) = Q(\psi, \psi)$ for all $\psi \in L^2(\mathbb{R}^{3N})$. By defintion, we have $Q(\varphi_\pi, \psi_\pi) = Q(\varphi, \psi)$, for all $\pi \in S_N$. Therefore, we find

$$\begin{aligned} Q(\psi_s, \psi - \psi_s) &= \frac{1}{N!^2} \sum_{\pi,\sigma} Q(\psi_\pi, \psi - \psi_\sigma) \\ &= \frac{1}{N!^2} \sum_{\pi,\sigma} Q(\psi, \psi_{\pi^{-1}} - \psi_{\pi^{-1}\sigma}) \\ &= Q(\psi, \psi_s - \psi_s) = 0 \end{aligned}$$

Writing $\mathcal{E}(\psi) = Q(\psi, \psi)$ and decomposing $\psi = \psi_s + \psi_r$, we obtain (3.25). Similarly, we also find

$$1 = \|\psi\|^2 = \|\psi_s\|^2 + \|\psi_r\|^2$$

Thus, we conclude

$$E_0 = \mathcal{E}(\psi) = \mathcal{E}(\psi_s) + \mathcal{E}(\psi_r) \geq E_0 \|\psi_s\|_2^2 + E_0 \|\psi_r\|^2 = E_0$$

and thus that $\mathcal{E}(\psi_s) = E_0 \|\psi_s\|^2$. Since $\|\psi_s\|_2 \neq 0$, it follows that $\mathcal{E}(\psi_s / \|\psi_s\|^2) = E_0$. If there is no minimizer, we can proceed similarly, using a minimizing sequence. □

**Corollary 3.0.4.** *Consider the Hamilton operator $H_{N,M}(\mathbf{R}, \mathbf{Z})$ defined in (3.19), for a system with $N$ electrons and $M$ static nuclei. Then unrestricted minimizers of $\mathcal{E}(\psi) = \langle \psi, H_{N,M}(\mathbf{R}, \mathbf{Z})\psi \rangle$ are bosonic. In other words,*

$$\begin{aligned} &\inf\{\langle \psi, H_{N,M}(\mathbf{R}, \mathbf{Z})\psi \rangle : \psi \in L^2(\mathbb{R}^{3N}), \|\psi\|_2 = 1\} \\ &\qquad = \inf\{\langle \psi, H_{N,M}(\mathbf{R}, \mathbf{Z})\psi \rangle : \psi \in L^2_s(\mathbb{R}^{3N}), \|\psi\|_2 = 1\} \end{aligned}$$

*Proof.* It is enough to show that the quadratic form $\mathcal{E}(\psi) = \langle \psi, H_{N,M}(\mathbf{R}, \mathbf{Z})\psi \rangle$ satisfies the assumptions of Proposition 3.0.3. Assumption i) is a consequence of stability of the first kind. Assumption iii) is easy to verify. As for assumption ii), it follows from the remark that

$$|\nabla \psi(x)|^2 \geq |\nabla |\psi(x)||^2$$

for almost all $x \in \mathbb{R}^d$ and any $\psi \in H^1(\mathbb{R}^d)$ (proof: exercise). □

## 3.1 Lieb-Thirring Inequalities

The Lieb-Thirring inequality provides an upper bound for the sum of the absolute value of the negative eigenvalues of $h = -\Delta + V$. More generally, it provides bounds for the sum of powers of the eigenvalues of $h$.

**Theorem 3.1.1.** *Fix $\gamma \geq 0$ and assume $V_- = \max(0, -V) \in L^{\gamma+3/2}(\mathbb{R}^d)$. Let $e_0 \leq e_1 \leq e_2 \leq \dots$ be the non-positive eigenvalues of $h = -\Delta + V$. There exists a constant $C = C(\gamma) > 0$, independent of $V$, such that*

$$\sum_{j \geq 0} |e_j|^\gamma \leq C \int_{\mathbb{R}^3} V_-(x)^{\gamma+3/2} dx \tag{3.26}$$

*Remark:* Observe that, for $\gamma = 0$, (3.26) gives an upper bound on the number of negative eigenvalues of the operator $h = -\Delta + V$.

*Proof.* We prove the theorem for $\gamma = 1$, which represents the most important case.
It is enough to show that

$$\sum_{j=1}^{N} \langle \phi_j, h\phi_j \rangle \geq -C \int V_-(x)^{5/2} dx \tag{3.27}$$

for all finite orthonormal families $\{\phi_j\}_{j=1}^N$ in $L^2(\mathbb{R}^d)$. We can choose $\varphi_j$ to be the eigenvectors associated with the negative eigenvalues of $h$.
For any $\phi \in L^2(\mathbb{R}^d)$ and $e > 0$, the decomposition $\phi = \phi^{e,+} + \phi^{e,-}$ holds true, with $\phi^{e,\pm}$ defined through Fourier transform by

$$\widehat{\phi^{e,+}}(p) = \widehat{\phi}(p)\chi(|p| > \sqrt{e}), \qquad \widehat{\phi^{e,-}}(p) = \widehat{\phi}(p)\chi(|p| \leq \sqrt{e})$$

By unitarity of the Fourier transform in $L^2(\mathbb{R}^d)$

$$\begin{aligned} \int_0^\infty \left[ \int |\phi^{e,+}(x)|^2 dx \right] de &= \int_0^\infty \left[ \int |\widehat{\phi^{e,+}}(p)|^2 dp \right] de = \int \left[ \int_0^\infty |\widehat{\phi^{e,+}}(p)|^2 de \right] dp \\ &= \int \left[ \int_0^{p^2} |\widehat{\phi}(p)|^2 de \right] dp = \int |p|^2 |\widehat{\phi}(p)|^2 dp = \int |\nabla \phi(x)|^2 dx \end{aligned} \tag{3.28}$$

Notice that, for any $j = 1, \ldots, N$, we have

$$|\phi_j(x)|^2 = |\phi_j^{e,+}(x) + \phi_j^{e,-}(x)|^2 \leq |\phi_j^{e,+}(x)|^2 + |\phi_j^{e,-}(x)|^2 + 2|\phi_j^{e,+}(x)||\phi_j^{e,-}(x)|.$$

Hence (exercise),

$$\sum_{j=1}^{N} |\phi_j(x)|^2 \leq \left[ \left( \sum_{j=1}^{N} |\phi_j^{e,+}(x)|^2 \right)^{1/2} + \left( \sum_{j=1}^{N} |\phi_j^{e,-}(x)|^2 \right)^{1/2} \right]^2$$

Thus

$$\left( \sum_{j=1}^{N} |\phi_j(x)|^2 \right)^{1/2} \leq \left( \sum_{j=1}^{N} |\phi_j^{e,+}(x)|^2 \right)^{1/2} + \left( \sum_{j=1}^{N} |\phi_j^{e,-}(x)|^2 \right)^{1/2}$$

which leads us to

$$\left( \sum_{j=1}^{N} |\phi_j^{e,+}(x)|^2 \right)^{1/2} \geq \left[ \left( \sum_{j=1}^{N} |\phi_j(x)|^2 \right)^{1/2} - \left( \sum_{j=1}^{N} |\phi_j^{e,-}(x)|^2 \right)^{1/2} \right]_+ \tag{3.29}$$

where we used the notation $s_+ = \max(0, s)$. Using the unitarity of the Fourier transform and Bessel's inequality, we obtain

$$\begin{aligned}\sum_{j=1}^N |\phi_j^{e,-}(x)|^2 &= \sum_{j=1}^N \left| \frac{1}{(2\pi)^{3/2}} \int e^{ip\cdot x} \widehat{\phi}_j(p) \chi(|p| \leq e^{1/2}) dp \right|^2 \\ &= \frac{1}{(2\pi)^3} \sum_{j=1}^N \left| \langle e^{i.\cdot x} \widehat{\chi(|.| \leq e^{1/2})}, \phi_j \rangle \right|^2 \\ &\leq \frac{1}{(2\pi)^3} \|\chi(|.| \leq e^{1/2})\|_2^2 = \frac{|S_2|}{(2\pi)^3} e^{3/2}\end{aligned} \tag{3.30}$$

Combining (3.28), (3.29), (3.30) yields

$$\sum_{j=1}^N \int |\nabla \phi_j(x)|^2 dx \geq \int \int_0^\infty \left[ \left( \sum_{j=1}^N |\phi_j(x)|^2 \right)^{1/2} - \frac{|S_2|^{1/2}}{(2\pi)^{3/2}} e^{3/4} \right]_+^2 de dx$$

With $e_0 = (2\pi)^2 |S_2|^{-2/3} (\sum_{j=1}^N |\phi_j(x)|^2)^{2/3}$, we obtain

$$\begin{aligned}\sum_{j=1}^N \int |\nabla \phi_j(x)|^2 dx &\geq \int \int_0^{e_0} \left[ \left( \sum_{j=1}^N |\phi_j(x)|^2 \right)^{1/2} - \frac{|S_2|^{1/2}}{(2\pi)^{3/2}} e^{3/4} \right]^2 de dx \\ &= \frac{(2\pi)^2}{|S_2|^{2/3}} \frac{9}{35} \int \left( \sum_{j=1}^N |\phi_j(x)|^2 \right)^{5/3} dx\end{aligned} \tag{3.31}$$

Hölder's inequality implies

$$\begin{aligned}\sum_{j=1}^N \langle \phi_j, H\phi_j \rangle &= \sum_{j=1}^N \int \left[ |\nabla \phi_j(x)|^2 + V(x) |\phi_j(x)|^2 \right] dx \geq \sum_{j=1}^N \int \left[ |\nabla \phi_j(x)|^2 - V_-(x) |\phi_j(x)|^2 \right] dx \\ &\geq \frac{(2\pi)^2}{|S_2|^{2/3}} \frac{9}{35} \int \left( \sum_{j=1}^N |\phi_j(x)|^2 \right)^{5/3} dx \\ &\quad - \left[ \int V_-(x)^{5/2} dx \right]^{2/5} \left[ \int \left( \sum_{j=1}^N |\phi_j(x)|^2 \right)^{5/3} dx \right]^{3/5}\end{aligned}$$

Finally, we use the fact that, for any parameter $a, b > 0$ and any $t \geq 0$,

$$at - bt^{3/5} \geq -\frac{2}{5} \left[ \frac{3}{5} \right]^{3/2} a^{-3/2} b^{5/2}$$

to conclude that

$$\sum_{j=1}^{N}\langle\phi_j, H\phi_j\rangle \geq -\frac{2}{5}\left(\frac{7}{3}\right)^{3/2}\frac{|S_2|}{(2\pi)^3}\int V_-(x)^{5/2}dx$$

This shows (3.27) and concludes the proof of the theorem (for the case $j = 1$). □

The following bounds for the expectation of the kinetic energy in a fermionic state are a simple consequence of the Lieb-Thirring inequality.

**Theorem 3.1.2.** *There exists a constant $C > 0$ such that, for every fermionic wave function $\psi \in L^2_a(\mathbb{R}^{dN})$ we have*

$$\left\langle\psi, \sum_{j=1}^{N} -\Delta_{x_j}\psi\right\rangle \geq C\int \rho_\psi^{5/3}(x)dx \tag{3.32}$$

*where*

$$\rho_\psi(x) = N\int |\psi_N(x, x_2, \ldots, x_N)|^2\, dx_2 \ldots dx_N$$

*is the density of particles close to $x \in \mathbb{R}^3$, in the state $\psi$. In other words, $\rho_\psi(x) = \gamma_\psi^{(1)}(x; x)$ is the diagonal of the one-particle reduced density associated with $\psi$.*

The proof is left as an exercise. Indeed, by the proof of the Lieb-Thirring inequality, decomposing the one-particle reduced density of $\psi$ in its spectral representation as $\gamma_\psi^{(1)} = \sum_j \lambda_j|\phi_j\rangle\langle\phi_j|$, with weights $0 \leq \lambda_j \leq 1$ satisfying $\sum \lambda_j = 1$ and with orthonormal wave functions $\phi_j \in L^2(\mathbb{R}^d)$, it is easy to check that (3.32) is equivalent to

$$\sum_j \lambda_j \int |\nabla\phi_j(x)|^2 dx \geq C\int \left(\sum_j \lambda_j|\phi_j(x)|^2\right)^{1+2/d} dx$$

which is a simple extension of (3.31).

**Remark 3.1.3.** *The fermionic symmetry of $\psi$ plays a crucial role in (3.32). For bosonic wave functions, we only have $0 \leq \gamma_\psi \leq N$, and thus (**??**) has to be replaced by the weaker estimate*

$$\langle\psi, H\psi\rangle \geq -CN\int V_-(x)^{5/2}dx$$

*leading to the bound*

$$\left\langle\psi, \sum_{j=1}^{N} -\Delta_{x_j}\psi\right\rangle \geq \frac{C}{N^{2/3}}\int \rho_\psi^{5/3}(x)dx.$$

## 3.2 Electrostatic Inequalities

We will now focus on the parts of the energy in which the Coulomb interaction appears and set the tools to bound its expectation from below. To this end we introduce the following objects:

**Definition 3.2.1.** *Let $\mu$ be a possibly signed Borel measure on $\mathcal{B}(\mathbb{R}^3)$. The potential associated with $\mu$ is given by*

$$\phi(x) = \int \frac{1}{|x-y|}\, d\mu(y). \tag{3.33}$$

Observe that if $\mu$ is a positive measure, $\phi$ is always well-defined, although it could be infinite. If $\mu = \sigma - \tau$ is a signed measure, given by the difference of two positive Borel measures $\sigma, \nu$, the potential is not necessarily well-defined because there could be cancellations between the contributions of $\sigma$ and $\nu$.
In the following, we will consider potentials associated with Borel measures of the form $\mu = \sigma - \nu$, with $\sigma, \nu$ positive Borel measures satisfying

$$\int \frac{1}{1+|x|} d\sigma(x), \int \frac{1}{1+|x|} d\nu(x) < \infty \tag{3.34}$$

**Definition 3.2.2.** *The Coulomb energy of a positive measure $\nu$ is defined as*

$$\mathcal{D}(\nu,\nu) = \frac{1}{2}\int \frac{1}{|x-y|} d\nu(x) d\nu(y)$$

**Definition 3.2.3.** *A charge distribution is a Borel measure $\mu = \sigma - \nu$, where $\sigma, \nu$ are positive Borel measure satisfying (3.34) and having finite Coulomb energy $\mathcal{D}(\sigma,\sigma), \mathcal{D}(\nu,\nu) < \infty$. We can then define the Coulomb energy of the charge distribution $\mu$ through*

$$\mathcal{D}(\mu,\mu) = \frac{1}{2}\int \frac{1}{|x-y|} d\mu(x) d\mu(y)$$

*More generally, given two charge distributions $\mu_1, \mu_2$, we can define their interaction energy*

$$\mathcal{D}(\mu_1,\mu_2) = \frac{1}{2}\int \frac{1}{|x-y|} d\mu_1(x) d\mu_2(y)$$

**Proposition 3.2.4.** *Let $\mu$ be a charge distribution. Then*

*i) $D(\mu,\mu) \geq 0$.*

*ii) For any two charge distributions $\mu_1, \mu_2$, we have*

$$D(\mu_1,\mu_2) \leq \sqrt{D(\mu_1,\mu_1)}\sqrt{D(\mu_2,\mu_2)}.$$

**Lemma 3.2.5.** *There exists a positive constant $C$ such that for $x, y \in \mathbb{R}^3$*

$$\frac{1}{|x-y|} = \frac{1}{C}\int \frac{dz}{|x-z|^2|y-z|^2} \tag{3.35}$$

*Proof.* Observe that

$$\int \frac{1}{|x-z|^2|y-z|^2}dz = \int \frac{1}{|z|^2|(x-y)-z|^2}dz$$

is only a function of $|x-y|$. W.l.o.g. we can therefore write $(x-y) = |x-y|e_3$, with $e_3 = (0,0,1)$. By a change of variables we get

$$\begin{aligned}\int \frac{1}{|x-z|^2|y-z|^2}dz &= \frac{1}{|x-y|^2}\int dz \frac{1}{|z|^2\left|\frac{z}{|x-y|}-e_3\right|^2} \\ &= \frac{1}{|x-y|}\int dz \frac{1}{|z|^2|z-e_3|^2} = \frac{C}{|x-y|}\end{aligned}$$

for an appropriate constant $C > 0$. □

*Proof of Proposition 3.2.4. i*) Using (3.35) and Fubini's theorem we obtain

$$D(\mu,\mu) = \int \frac{1}{|x-y|}d\mu(x)d\mu(y) = \frac{1}{C}\int dz \left|\int \frac{1}{|x-z|^2}d\mu(x)\right|^2 \geq 0$$

*ii*) Exercise. □

An important property of Coulomb potentials of the form (3.33) is that, for spherically symmetric charges, they can be often controlled by the potential generated by a pointwise charge. More precisely, we have the following Newton's theorem.

**Theorem 3.2.6.** *Let $\mu$ be a charge distribution, invariant w.r.t. rotations. Then*

$$\phi(x) = \int \frac{1}{|x-y|}d\mu(y) = \frac{1}{|x|}\int_{|y|<|x|} d\mu(y) + \int_{|y|>|x|} \frac{1}{|y|}\,d\mu(y) \tag{3.36}$$

**Corollary 3.2.7.** *If supp $\mu \subset B_R(0)$ (meaning that $\mu(A) = 0$ for all $A \subset B_R(0)^c$), we find*

$$\phi(x) = \frac{\mu(\mathbb{R}^3)}{|x|}$$

*for all $|x| > R$.*
*If $\mu(\{y \in \mathbb{R}^3 : |y| < R\}) = 0$, then*

$$\phi(x) = \int_{|y|>R} \frac{1}{|y|}d\mu(y)$$

*for all $|x| < R$ (hence $\phi$ is constant on $|x| < R$).*
*If $\mu$ is a positive measure, (3.36) also implies that*

$$\phi(x) \leq \frac{\mu(\mathbb{R}^3)}{|x|} \tag{3.37}$$

*for all $x \in \mathbb{R}^3$.*

*Proof of Theorem 3.2.6.* Since $\phi(Rx) = \phi(x)$ for all $R \in SO(3)$, it follows easily that

$$\begin{aligned}\phi(x) &= \frac{1}{4\pi}\int_{S^2} d\omega\, \phi(|x|\omega) \\ &= \frac{1}{4\pi}\int d\mu(y)\int_{S^2} d\omega \frac{1}{|y-|x|\omega|} = \frac{1}{4\pi}\int d\mu(y)\int_{S^2} d\omega \frac{1}{||y|e_3-|x|\omega|}\end{aligned}$$

We focus on the integral in $d\omega$ and compute it explicitly:

$$\begin{aligned}\int_{S^2}\frac{1}{||y|e_3-|x|\omega|}\,d\omega &= \int_0^\pi \sin\theta \int_0^{2\pi} \frac{1}{\sqrt{|x|^2\sin^2\theta + (|x|\cos\theta - |y|)^2}}\,d\varphi\,d\theta \\ &= 2\pi\int_0^\pi \frac{\sin\theta}{\sqrt{|x|^2+|y|^2-2|x||y|\cos\theta}}d\theta \\ &= \frac{2\pi}{|x||y|}\left(||x|+|y||-||x|-|y||\right) = \frac{2\pi}{|x||y|}\begin{cases} 2|x| & \text{if } |x|<|y| \\ 2|y| & \text{if } |y|\le|x| \end{cases}\end{aligned}$$

Thus

$$\phi(x) = \frac{1}{|x|}\int_{|y|\le|x|} d\mu(y) + \int_{|x|<|y|}\frac{1}{|y|}d\mu(y)$$

□

We are now ready to state and prove the Electrostatic Inequality, that will be used to estimate the energy of an electron due to the interaction with all nuclei, excluding the closest one.

**Theorem 3.2.8.** *For any charge distribution $\mu$ and for every set of points $R_1,\dots,R_M \in \mathbb{R}^3$, we have*

$$D(\mu,\mu) - \int \phi(x)d\mu(x) + \sum_{k<\ell}^{M}\frac{Z^2}{|R_k-R_\ell|} \ge \frac{Z^2}{8}\sum_{j=1}^{M}\frac{1}{D_j},$$

*where*

$$D_j = \frac{1}{2}\min_{i\neq j}|R_i - R_j|.$$

Before proving the theorem we define few useful objects.

**Definition 3.2.9.** *Let $R_1,\dots,R_M$ be $M$ distinct nuclei in $\mathbb{R}^3$. We define the cell $\Gamma_j \subset \mathbb{R}^3$ by*

$$\Gamma_j = \{x\in\mathbb{R}^3 : |x-R_j| < |x-R_i| \text{ for all } i\neq j\}$$

Notice that $\Gamma_j$ is the set of points in $\mathbb{R}^3$ that are closer to $R_j$ than to any other $R_i$, $i\neq j$. By definition $\Gamma_j$ is open and convex. Its boundary $\partial\Gamma_j$ consists of a finite collection of plane segments. Moreover, $D_j$ can be interpreted as the distance from $R_j$ to $\partial\Gamma_j$.

**Definition 3.2.10.** *The potential produced by the nuclear configuration $R_1,\dots,R_M$ with equal charges $Z$ at $x$ is given by*

$$W(x) = Z\sum_{k=1}^{M}\frac{1}{|x-R_k|}$$

Observe that $W$ is harmonic on $\mathbb{R}^3\backslash\{R_1,\dots,R_M\}$. Let

$$\mathcal{D}(x)=\min\{|x-R_i|:1\le i\le M\}$$

be the distance from $x$ to the closest nucleus. By definition, we have $\mathcal{D}(x)=|x-R_j|$ for all $x\in\Gamma_j$. We set

$$\phi(x)=W(x)-\frac{Z}{\mathcal{D}(x)}$$

for all $x\in\mathbb{R}^3$. For $x\in\Gamma_j$, $\phi(x)$ is the potential generated at $x\in\Gamma_j$ by all nuclei outside $\Gamma_j$. We observe that $\phi$ is a continuous functions on $\mathbb{R}^3$, harmonic in each cell $\Gamma_j$, but not harmonic on $\mathbb{R}^3$ (exercise).

*Proof.* We divide the proof into three steps.
Step 1. Find a charge distribution $\nu$ generating the potential $\phi$, i.e.

$$\phi(x)=\int\frac{1}{|x-y|}d\nu(y)$$

that is $-\Delta\phi=4\pi\nu$. To this end let $f\in C_c^\infty(\mathbb{R}^3)$ be a test function and compute

$$\begin{aligned}4\pi\int f(x)d\nu(x)&=-\int\phi(x)\Delta f(x)dx=-\sum_{j=1}^M\int_{\Gamma_j}\phi(x)\Delta f(x)dx\\&=-\sum_{j=1}^M\int_{\Gamma_j}\nabla\cdot(\phi(x)\nabla f(x))dx+\sum_{j=1}^M\int_{\Gamma_j}\nabla\phi(x)\cdot\nabla f(x)dx\\&=-\sum_{j=1}^M\int_{\partial\Gamma_j}\phi(x)\nabla f(x)\cdot n_j d\sigma+\sum_{j=1}^M\int_{\Gamma_j}\nabla\phi(x)\cdot\nabla f(x)dx\end{aligned}\tag{3.38}$$

Since $\nabla f$ and $\phi$ are continuous and every segment in $\partial\Gamma_j$ appears twice with opposite sign, the first term on the r.h.s of (3.38) is zero. We are therefore left with

$$\sum_{j=1}^M\int_{\Gamma_j}\nabla f(x)\cdot\nabla\phi(x)dx=\sum_{j=1}^M\int_{\Gamma_j}\nabla\cdot(f(x)\nabla\phi(x))\,dx-\sum_{j=1}^M\int_{\Gamma_j}f(x)\Delta\phi(x)dx$$

Since $\Delta\phi=0$ inside every cell $\Gamma_j$, we arrive at

$$\sum_{j=1}^M\int_{\Gamma_j}\nabla f(x)\cdot\nabla\phi(x)dx=\sum_{j=1}^M\int_{\partial\Gamma_j}f(x)\nabla\phi(x)\cdot n_j d\sigma$$

We conclude that

$$4\pi\int f(x)d\nu(x)=\sum_{j=1}^M\int_{\partial\Gamma_j}f(x)\nabla\phi(x)\cdot n_j d\sigma\tag{3.39}$$

As before, every segment $\partial\Gamma_j$ appears twice with opposite signs, but the integral is not zero because $\nabla\phi$ is not continuous on$\partial\Gamma_j$. We now recall that

$$\phi(x) = W(x) - \frac{Z}{\mathcal{D}(x)}$$

Since $W$ is differentiable on $\partial\Gamma_j$, its contribution to the r.h.s. of (3.39) vanishes. On the segment $\partial\Gamma_j \cap \partial\Gamma_\ell$, we have

$$n_j \cdot \nabla \frac{1}{|x - R_j|} = n_\ell \cdot \nabla \frac{1}{|x - R_\ell|}$$

and thus

$$-4\pi \int f(x) d\nu(x) = 2Z \int_{\bigcup_j \partial\Gamma_j} f(x)\, n_j \cdot \nabla \frac{1}{|x - R_j|} d\sigma(x)$$

Hence $\nu$ is a surface charge density concentrated on the boundaries $\cup_j \partial\Gamma_j$. On the segment $\partial\Gamma_j \cap \partial\Gamma_\ell$, it holds

$$-\frac{Z}{2\pi} n_j \cdot \nabla \frac{1}{|x - R_j|} = -\frac{Z}{2\pi} n_\ell \cdot \nabla \frac{1}{|x - R_\ell|}$$

Moreover,

$$-n_j \cdot \nabla \frac{1}{|x - R_j|} = n_j \cdot \frac{(x - R_j)}{|x - R_j|^3} \geq 0$$

by the convexity of $\Gamma_j$, yielding to $\nu$ being a positive measure. We can therefore write

$$\int \phi(x) d\mu(x) = \int \frac{1}{|x - y|} d\nu(y) d\mu(x) = 2D(\mu, \nu) = 2D(\nu, \mu)$$

*Step 2.* Plugging this into the expression we want to bound yields

$$\begin{aligned} D(\mu, \mu) - \int \phi(x) d\mu(x) + \sum_{k<\ell}^{M} \frac{Z^2}{|R_k - R_\ell|} &= D(\mu - \nu, \mu - \nu) - D(\nu, \nu) + \sum_{k<\ell}^{M} \frac{Z^2}{|R_k - R_\ell|} \\ &\geq -D(\nu, \nu) + \sum \frac{Z^2}{|R_k - R_\ell|} \end{aligned} \tag{3.40}$$

because $D(\mu - \nu, \mu - \nu) \geq 0$ by positivity of the Coulomb energy.
*Step 3.* To conclude the proof, we compute $D(\nu, \nu)$. To this end, we notice that

$$W(x) = Z \sum_{j=1}^{M} \frac{1}{|x - R_j|} = Z \sum_{j=1}^{N} \int_{\mathbb{R}^3} \frac{1}{|y - x|} \delta(y - R_j) dy$$

Thus

$$\int W(x) \nu(dx) = Z \sum_{j=1}^{M} \int_{\mathbb{R}^3} dy\, \delta(y - R_j) \int d\nu(x) \frac{1}{|x - y|} = Z \sum_{j=1}^{M} \phi(R_j) = 2Z^2 \sum_{k<\ell}^{M} \frac{1}{|R_k - R_\ell|}$$

Hence

$$D(\nu,\nu) = \frac{1}{2}\int \frac{1}{|x-y|}d\nu(x)d\nu(y) = \frac{1}{2}\int \phi(x)d\nu(x) = \frac{1}{2}\int W(x)d\nu(x) - \frac{Z}{2}\int \frac{1}{\mathcal{D}(x)}d\nu(x)$$
$$= Z^2\sum_{k<\ell}^{M}\frac{1}{|R_k - R_\ell|} - \frac{Z}{2}\int \frac{1}{\mathcal{D}(x)}d\nu(x)$$

From (3.40), we conclude that

$$D(\mu,\mu) - \int \phi(x)d\mu(x) + \sum_{k<\ell}^{M}\frac{Z^2}{|R_k - R_\ell|}$$
$$\geq \frac{Z}{2}\int \frac{1}{\mathcal{D}(x)}d\nu(x) = -\frac{Z^2}{8\pi}\sum_{j=1}^{M}\int_{\partial\Gamma_j}\frac{1}{\mathcal{D}(x)}n_j\cdot\nabla\frac{1}{|x-R_j|}d\sigma$$
$$= -\frac{Z^2}{8\pi}\sum_{j=1}^{M}\int_{\partial\Gamma_j}\frac{1}{|x-R_j|}n_j\cdot\nabla\frac{1}{|x-R_j|}d\sigma$$
$$= -\frac{Z^2}{16\pi}\sum_{j=1}^{M}\int_{\partial\Gamma_j} n_j\cdot\nabla\frac{1}{|x-R_j|^2}d\sigma = \frac{Z^2}{16\pi}\sum_{j=1}^{M}\int_{\Gamma_j^c}\Delta\frac{1}{|x-R_j|^2}dx$$
$$= \frac{Z^2}{8\pi}\sum_{j=1}^{M}\int_{\Gamma_j^c}\frac{1}{|x-R_j|^4}dx$$

Since the integrand is positive, the integral over $\Gamma_j^c$ is larger than if we integrate over the whole half-plane defined by the prolongation of the segment of $\partial\Gamma_j$ at distance $D_j$ from $R_j$. Hence

$$D(\mu,\mu) - \int \phi(x)d\mu(x) + \sum_{k<\ell}^{M}\frac{Z^2}{|R_k - R_\ell|}$$
$$\geq \frac{Z^2}{8\pi}\sum_{j=1}^{M}\int_{\mathbb{R}}dy\int_{\mathbb{R}}dz\int_{D_j}^{\infty}\frac{1}{(x^2+y^2+z^2)^2}dx$$
$$= \frac{Z^2}{4}\sum_{j=1}^{M}\int_0^\infty rdr\int_{D_j}^{\infty}dx\,\frac{1}{(r^2+x^2)^2} = \frac{Z^2}{8}\sum_{j=1}^{M}\int_{D_j}^{\infty}\frac{1}{x^2}dx = \frac{Z^2}{8}\sum_{j=1}^{M}\frac{1}{D_j}$$

□

As an application of the basic electrostatic inequality (Theorem 3.2.8), we can show a pointwise bound on the potential energy of $N$ electrons interacting with $M$ nuclei, all having charge $Z$, known as Baxter's inequality.

**Theorem 3.2.11.** *Let*

$$V(\mathbf{x},\mathbf{R}) = \sum_{i<j}^{N} \frac{1}{|x_i - x_j|} - \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{Z}{|x_i - R_j|} + \sum_{k<\ell}^{M} \frac{Z^2}{|R_k - R_\ell|}$$

*As above, we denote by* $\Gamma_j \subset \mathbb{R}^3$ *the Voronoi cell with* $R_j$, $\mathcal{D}(x) = \min\{|x - R_j|, j = 1, \dots, M\}$ *and* $D_j = \min\{|R_i - R_j|/2, i \neq j\}$. *Then*

$$V(\mathbf{x},\mathbf{R}) \geq -(2Z+1)\sum_{j=1}^{M} \frac{1}{\mathcal{D}(x_j)} + \frac{Z^2}{8}\sum_{j=1}^{M} \frac{1}{D_j}$$

*Proof.* Exercise. □

## 3.3 Indirect Part of the Coulomb Energy

For any antisymmetrix wave function $\psi_N \in L^2_a(\mathbb{R}^{3N})$, we define

$$I_{\psi_N} = \left\langle \psi_N, \sum_{i<j}^{N} \frac{1}{|x_i - x_j|}\psi_N \right\rangle = \sum_{i<j}^{N} \int dx_1 \dots dx_N \frac{1}{|x_i - x_j|}|\psi_N(x_1, \dots, x_N)|^2$$

Recall the definition of space density associated with a wave funciton $\psi_N$

$$\rho_{\psi_N}(x) = N \int dx_2 \dots dx_N \, |\psi_N(x, x_2, \dots, x_N)|^2$$

such that $\int \rho_\psi(x)dx = N$. Notice that this definition implies $\rho_\psi(x) = \gamma^{(1)}(x;x)$, where $\gamma^{(1)}$ is the one-particle reduced density matrix associated with $\psi_N$. Hence, the electrostatic energy associated with the electron density $\rho_{\psi_N}$ is given by

$$D(\rho_\psi, \rho_\psi) = \frac{1}{2}\int dxdy \, \frac{\rho_\psi(x)\rho_\psi(y)}{|x-y|}$$

We observe that if $\psi \in L^2(\mathbb{R}^3)$ were a product, $I_\psi = D(\rho_\psi, \rho_\psi)$ because the two-particle reduced density that is needed to compute $I_\psi$ would be the product of two copies of the one-particle reduced density. The product wave functions describe situations in which particles are independent, so that the probability to find a particle at $x_i$ and a particle at $x_j$ is given simply by the product of the two probabilities. From this interpretation, it follows that the difference between $I_\psi$ and $D(\rho_\psi, \rho_\psi)$ is related to the correlation among particles. Such correlations may be caused by the interaction among particles or by the antisymmetric nature of the wave function, which has therefore a built in correlation structure. The next theorem provides a lower bound on such correlations, i.e. on the difference $I_\psi - D(\rho_\psi, \rho_\psi)$, known as the indirect part of the Coulomb energy, as opposite to $D(\rho_\psi, \rho_\psi)$ known as the direct part of the Coulomb energy.

**Theorem 3.3.1.** *For every* $\psi_N \in L^2_a(\mathbb{R}^{3N})$, *we have*

$$I_{\psi_N} - D(\rho_{\psi_N}, \rho_{\psi_N}) \geq -C \int \rho^{4/3}_{\psi_N}(x)dx$$

*Proof.* The proof is divided into several intermediate steps.

*Step 1.* For any $z \in \mathbb{R}^3$, let $\mu_z$ be a non-negative, spherical symmetric w.r.t. $z$, bounded function with

$$\int \mu_z(y)dy = 1$$

Then for every $\rho \in L^1(\mathbb{R}^3)$ non-negative, we have

$$\sum_{i<j}^{N} \frac{1}{|x_i - x_j|} \geq -D(\rho,\rho) + 2\sum_{i=1}^{N} D(\rho, \mu_{x_i}) - \sum_{i=1}^{N} D(\mu_{x_i}, \mu_{x_i}) \tag{3.41}$$

(the proof of (3.41) is an exercise).

*Step 2.* We have

$$I_\psi - D(\rho_\psi, \rho_\psi) \geq -F_1 - F_2 \tag{3.42}$$

with

$$F_1 = \int \frac{\rho_\psi(x)(\delta_z(y) - \mu_z(y))}{|x-y|}\rho_\psi(z)dxdydz$$

and

$$F_2 = \frac{1}{2}\int \frac{\mu_z(x)\mu_z(y)}{|x-y|}\rho_\psi(z)dxdydz$$

for any $\mu$ as in Step 1.

To show (3.42), we choose $\rho = \rho_\psi$ and we apply Step 1. We find

$$\begin{aligned} I_\psi = \Big\langle \psi, \sum_{i<j}^{N} \frac{1}{|x-y|}\psi \Big\rangle &\geq -D(\rho_\psi,\rho_\psi) + 2\sum_{j=1}^{N} \int |\psi(x_1,\dots,x_N)|^2 \, D(\rho_\psi, \mu_{x_j})\, dx_1 \dots dx_N \\ &\quad - \sum_{j=1}^{N} \int |\psi(x_1,\dots,x_N)|^2 \, D(\mu_{x_j}, \mu_{x_j})\, dx_1 \dots dx_N \\ &= -D(\rho_\psi,\rho_\psi) + 2\int \rho_\psi(z) D(\rho_\psi, \mu_z)\, dz - \int \rho_\psi(z) D(\mu_z, \mu_z)\, dz \end{aligned}$$

Hence

$$I_\psi - D(\rho_\psi,\rho_\psi) \geq -2D(\rho_\psi,\rho_\psi) + 2\int \rho_\psi(z) D(\rho_\psi, \mu_z)\, dz - \int \rho_\psi(z) D(\mu_z,\mu_z)\, dz$$

Note that

$$\begin{aligned} \int \rho_\psi(z) D(\rho_\psi, \delta_z)\, dz &= \frac{1}{2}\int \rho_\psi(z) \int \frac{\rho_\psi(x)\delta_z(y)}{|x-y|}\, dxdydz \\ &= \frac{1}{2}\int \frac{\rho_\psi(x)\rho_\psi(y)}{|x-y|}\, dxdy = D(\rho_\psi,\rho_\psi) \end{aligned}$$

It follows that

$$I_\psi - D(\rho_\psi, \rho_\psi) \geq -2 \int \rho_\psi(z) D(\rho_\psi, \delta_z - \mu_z)\, dz - \int \rho_\psi(z) D(\mu_z, \mu_z)\, dz = -F_1 - F_2$$

*Step 3.* Suppose now $\widetilde{\mu} \geq 0$ is bounded and such that $\int \widetilde{\mu}(x)dx = 1$ and $\widetilde{\mu}(x) = 0$ if $|x| > 1$. Set

$$\mu_z(x) = \rho_\psi(z)\widetilde{\mu}(\rho_\psi^{1/3}(z)(x-z)) \tag{3.43}$$

Then

$$F_2 = C \int \rho_\psi(y)^{4/3} dy\,. \tag{3.44}$$

The proof of (3.44) is left as an exercise.

*Step 4.* With the same choice of $\mu_z$ as in Step 3, we have

$$F_1 \leq C \int \rho_\psi^{4/3}(x) dx \tag{3.45}$$

To show (3.45), we compute

$$\begin{aligned} F_1 &= \int \rho_\psi(z)\, \frac{\rho_\psi(x)}{|x-y|} \left[\delta(z-y) - \rho_\psi(z)\widetilde{\mu}(\rho_\psi^{1/3}(z)(z-y))\right] dxdydz \\ &= \int \frac{\rho_\psi(x)\rho_\psi(y)}{|x-y|} dxdy - \int \rho_\psi(x)\rho_\psi(z) \int\ \rho_\psi(z) \frac{\widetilde{\mu}(\rho_\psi^{1/3}(z)(z-y))}{|x-y|} dxdydz \end{aligned}$$

We observe that

$$\begin{aligned} &\int \rho_\psi(x)\rho_\psi(z) \int \rho_\psi(z) \frac{\widetilde{\mu}(\rho_\psi^{1/3}(z)(z-y))}{|x-y|} dxdydz \\ &\qquad = \int \rho_\psi(x)\rho_\psi^{4/3}(z) \int d\widetilde{y} \frac{\widetilde{\mu}(y)}{|\rho_\psi^{1/3}(z)(x-z) - \widetilde{y}|} dxdydz \\ &\qquad = \int \rho_\psi(x)\rho_\psi^{4/3}(z)\phi(\rho^{1/3}(z)|x-z|)\, dxdz \end{aligned}$$

where we introduced the notation

$$\phi(t) = \int \frac{\widetilde{\mu}(y)}{|y-t|} dt$$

for the potential generated by $\widetilde{\mu}$. We obtain

$$F_1 = \int \frac{\rho_\psi(x)\rho_\psi(y)}{|x-y|} dxdy - \int \rho_\psi(x)\rho_\psi^{4/3}(y)\phi(\rho^{1/3}(z)|x-z|) dxdydz = \int \rho_\psi(x) R(\rho_\psi(y), |x-y|) dxdy$$

with

$$R(a,r) = \frac{a}{r} - a^{4/3}\phi(a^{1/3}r)$$

Since $\widetilde{\mu}$ is spherically symmetric, Newton's theorem implies that $\phi(r) \leq 1/r$. Thus $R(a,r) \geq 0$. Moreover, $R(a,r) = 0$ if $a^{1/3}r \geq 1$. We conclude that

$$0 \leq R(a,r) \leq \begin{cases} a/r & \text{if } a^{1/3}r < 1 \\ 0 & \text{if } a^{1/3}r \geq 1 \end{cases}$$

which implies that

$$F_1 \leq \int_{\rho^{1/3}(y)|x-y|\leq 1} \frac{\rho_\psi(x)\rho_\psi(y)}{|x-y|} dxdy$$

We use the representation

$$\rho_\psi(x) = \int_0^\infty \chi(\rho_\psi(x) \geq \alpha) d\alpha$$

With $\chi_\alpha(x) = \chi(\rho_\psi(x) \geq \alpha)$, we find

$$\begin{aligned} F_1 &\leq \int_0^\infty d\alpha \int_0^\infty d\beta \int_{\beta^{1/3}|x-y|\leq 1} dxdy \frac{\chi_\alpha(x)\chi_\beta(y)}{|x-y|} \\ &\leq \int_0^\infty d\alpha \int_0^\alpha d\beta \int_{\beta^{1/3}|x-y|\leq 1} dxdy \, \frac{\chi_\alpha(x)}{|x-y|} + \int_0^\infty d\alpha \int_\alpha^\infty d\beta \int_{\beta^{1/3}|x-y|\leq 1} dxdy \frac{\chi_\beta(y)}{|x-y|} \\ &=: \mathrm{I} + \mathrm{II} \end{aligned}$$

We estimate

$$\begin{aligned} \mathrm{I} &= \int_0^\infty d\alpha \int_0^\alpha d\beta \left[ \int_{|y|\leq \beta^{-1/3}} \frac{dy}{|y|} \right] \left[ \int \chi_\alpha(x) dx \right] \\ &\leq 2\pi \int_0^\infty d\alpha \int_0^\alpha d\beta \beta^{-2/3} \int \chi_\alpha(x) dx = 6\pi \int_0^\infty d\alpha \alpha^{1/3} \int \chi_\alpha(x) dx \end{aligned}$$

and

$$\begin{aligned} \mathrm{II} &= 2\pi \int_0^\infty d\alpha \int_\alpha^\infty d\beta \beta^{-2/3} \int dy \chi_\beta(y) = 2\pi \int_0^\infty d\alpha \int dy \int_\alpha^\infty d\beta \beta^{-2/3} \chi(\rho_\psi(y) \geq \beta) \\ &= 2\pi \int_0^\infty d\alpha \int dy \, \chi(\rho_\psi(y) \geq \alpha) \int_\alpha^{\rho_\psi(y)} d\beta \, \beta^{-2/3} \\ &= 6\pi \int_0^\infty d\alpha \int dy \chi_\alpha(y) (\rho_\psi^{1/3}(y) - \alpha^{1/3}) \end{aligned}$$

From the last two bounds, we conclude that

$$F_1 \leq \mathrm{I} + \mathrm{II} = 6\pi \int_0^\infty d\alpha \int dy \rho_\psi^{1/3}(y) \chi_\alpha(y) = C \int dy \rho_\psi^{4/3}(y)$$

□

## 3.4 Proof of Stability

We are going to give two proofs of (3.23). First of all, we recall notations that will be used. Let $N, M \in \mathbb{N}$, $\mathbf{R} = (R_1, \ldots, R_M) \in \mathbb{R}^{3M}$, $\mathbf{Z} = (Z_1, \ldots, Z_M) \in \mathbb{R}_+^M$. Let $\mathbf{x} \in \mathbb{R}^{3N}$. Then we define

$$V(\mathbf{R}, \mathbf{Z}, \mathbf{x}) = \sum_{i<j}^{N} \frac{1}{|x_i - x_j|} + \sum_{i<j}^{M} \frac{Z_i Z_j}{|R_i - R_j|} - \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{Z_i}{|x_i - R_j|}$$

and the Hamilton operator

$$H_{N,M}(\mathbf{R}, \mathbf{Z}) = \sum_{j=1}^{N} -\Delta_{x_j} + V(\mathbf{R}, \mathbf{Z}, \mathbf{x}) \tag{3.46}$$

acting as a self-adjoint operator on the space $L_a^2(\mathbb{R}^{3N})$.

We can also give a second proof of stability of the second kind.

**Theorem 3.4.1.** *There exists $C > 0$ with*

$$\inf_{\mathbf{R}} \inf_{\psi \in L_a^2(\mathbb{R}^{3N}) : \|\psi\|_2 = 1} \langle \psi, H_{N,M}(\mathbf{R}, \mathbf{Z}) \psi \rangle \geq -CN(1 + Z^2(N/M)^{2/3})$$

*Proof.* Again, by Prop. 3.0.2, it is enough to consider the case $Z_1 = \cdots = Z_M = Z$. From the kinetic energy inequality, Theorem 3.1.2, and the estimate for the indirect Coulomb energy, Theorem 3.3.1, we find

$$\begin{aligned} \langle \psi, H_{N,M}(\mathbf{R}, \mathbf{Z}) \psi \rangle \geq C \int \rho_\psi(x)^{5/3} dx + D(\rho_\psi, \rho_\psi) - C \int \rho_\psi^{4/3}(x) dx \\ - \sum_{j=1}^{M} \int \frac{Z}{|x - R_i|} \rho_\psi(x) dx + \sum_{i<j}^{M} \frac{Z^2}{|R_i - R_j|} \end{aligned}$$

With the basic electrostatic inequality, Theorem 3.2.8, we obtain

$$\langle \psi, H_{N,M}(\mathbf{R}, \mathbf{Z}) \psi \rangle \geq C \int \rho_\psi(x)^{5/3} dx - C \int \rho_\psi^{4/3}(x) dx - C \int \frac{Z}{\mathcal{D}(x)} \rho_\psi(x) dx$$

We bound now

$$\rho_\psi^{4/3}(x) = \rho_\psi(x) \rho_\psi^{1/3}(x) \leq a \rho_\psi^{5/3}(x) + a^{-1} \rho_\psi(x)$$

(the simple proof is left as an exercise).
Thus, choosing $a > 0$ small enough,

$$\langle \psi, H_{N,M}(\mathbf{R}, \mathbf{Z}) \psi \rangle \geq C \int \rho_\psi(x)^{5/3} dx - CZ \int \left[ \frac{1}{\mathcal{D}(x)} - b \right]_+ \rho_\psi(x) dx - CN - CZbN$$

With Hölder, we conclude that

$$\begin{aligned}\langle\psi, H_{N,M}(\mathbf{R},\mathbf{Z})\psi\rangle \geq & -CN(1+bZ)+C\int \rho_\psi^{5/3}(x)dx \\ & -CZ\left(\int\left[\frac{1}{\mathcal{D}(x)}-b\right]_+^{5/2}dx\right)^{2/5}\left(\int\rho_\psi^{5/3}(x)dx\right)^{3/5}\end{aligned}$$

Minimizing over all possible $\rho_\psi$, using namely that

$$\inf_{t>0} t - at^{3/5} = -Ca^{5/2}$$

Computing

$$\begin{aligned}\int\left[\frac{1}{\mathcal{D}(x)}-b\right]_+^{5/2}dx &\leq \sum_{j=1}^M\int\left(\frac{1}{|x-R_j|}-b\right)_+^{5/2}dx \\ &\leq \sum_{j=1}^M\int_{|x-R_j|<1/b}\left(\frac{1}{|x-R_j|}-b\right)^{5/2}dx \\ &= M\int_{|x|<1/b}(|x|^{-1}-b)^{5/2}dx = Mb^{5/2}\int_{b|x|\leq 1}\left[\frac{1}{b|x|}-1\right]^{5/2}dx \\ &= Mb^{-1/2}\int_{|y|\leq 1}\left[\frac{1}{|y|}-1\right]^{5/2}dy = CMb^{-1/2}\end{aligned} \tag{3.47}$$

we obtain

$$\begin{aligned}\langle\psi, H_{N,M}(\mathbf{R},\mathbf{Z})\psi\rangle &\geq -CN(1+bZ)-CZ^{5/2}\int\left[\frac{1}{\mathcal{D}(x)}-b\right]_+^{5/2}dx \\ &\geq -CN(1+bZ)-CZ^{5/2}Mb^{-1/2}\end{aligned}$$

Minimizing over $b>0$, we conclude that

$$\langle\psi, H_{N,M}(\mathbf{R},\mathbf{Z})\psi\rangle \geq -CN(1+Z^2(M/N)^{2/3})$$

Again by Young's inequality we obtain

$$\langle\psi, H_{N,M}(\mathbf{R},\mathbf{Z})\psi\rangle \geq -C(N+M)$$

where $C>0$ depends only on $Z$. □

# A Mathematical Background

## A.1 $L^p$ spaces and Hilbert spaces

Let $(\Omega,\mathcal{A},\mu)$ be a measure space, where $\Omega$ is a set, $\mathcal{A}$ a $\sigma$-algebra on $\Omega$ and $\mu$ a measure on the $\sigma$-algebra $\mathcal{A}$. For $1\leq p<\infty$, let

$$\mathcal{L}^p(\Omega,\mathcal{A},\mu)=\left\{f:\Omega\to\mathbb{C}\quad \mathcal{A}\text{-measurable s.t. }\int|f|^p d\mu<\infty\right\}$$

and, $f \in \mathcal{L}^p(\Omega, \mathcal{A}, \mu)$,

$$\|f\|_p = \left[\int |f|^p d\mu\right]^{1/p}.$$

For $p = \infty$, let

$$\mathcal{L}^\infty(\Omega, \mathcal{A}, \mu) = \{f : \Omega \to \mathbb{C} \text{ measurable s.t. } \exists\, C > 0 \text{ with } |f(x)| \leq C \text{ almost everywhere}\}$$

and, for $f \in \mathcal{L}^p(\Omega, \mathcal{A}, \mu)$ let

$$\|f\|_\infty = \inf\{C > 0 : |f(x)| \leq C \text{ almost everywhere}\}.$$

Hence $\|.\|_p : \mathcal{L}^p(\Omega, \mathcal{A}, \mu) \to [0; \infty)$, for any $1 \leq p \leq \infty$

$$\|\lambda f\|_p = |\lambda| \|f\|_p,$$

for all $\lambda \in \mathbb{C}$ and all $f \in \mathcal{L}^p(\Omega, \mathcal{A}, \mu)$. Moreover, for all $f, g \in \mathcal{L}^p(\Omega, \mathcal{A}, \mu)$ the triangular inequality holds:

$$\|f + g\|_p \leq \|f\|_p + \|g\|_p, \tag{A.48}$$

Nevertheless, $\|.\|_p$ does not define a norm on the vector space $\mathcal{L}^p(\Omega, \mathcal{A}, \mu)$, because $\|f\|_p = 0$ does not imply that $f = 0$ (it only implies that $f(x) = 0$ almost everywhere).
To make $\|.\|_p$ into a norm, we define the following equivalence relation on $\mathcal{L}^p(\Omega, \mathcal{A}, \mu)$, an equivalence relation. For $f, g \in \mathcal{L}^p(\Omega, \mathcal{A}, \mu)$ we write

$$f \sim g \text{ if and only if } f(x) = g(x) \ \mu\text{-almost everywhere.}$$

We can therefore define, for any $1 \leq p \leq \infty$,

$$L^p(\Omega, \mathcal{A}, \mu) = \mathcal{L}^p(\Omega, \mathcal{A}, \mu)/\sim = \{[f] : f \in \mathcal{L}^p(\Omega, \mathcal{A}, \mu)\}$$

where $[f] = \{g \in \mathcal{L}^p(\Omega, \mathcal{A}, \mu) : g \sim f\}$ is the equivalence class associated with $f$, which contains all functions that coincide with $f$ almost everywhere. Switching from $\mathcal{L}^p(\Omega, \mathcal{A}, \mu)$ to $L^p(\Omega, \mathcal{A}, \mu)$, we make the space smaller, because we identify functions that coincide almost everywhere. By definition, elements of $L^p(\Omega, \mathcal{A}, \mu)$ are not functions, they are equivalence classes of functions.
On $L^p(\Omega, \mathcal{A}, \mu)$ we can define the structure of a vector space, by setting

$$[f] + [g] = [f + g], \qquad \lambda[f] = [\lambda f]$$

We can also define $\|.\|_p : L^p(\Omega, \mathcal{A}, \mu) \to [0; \infty)$ through $\|[f]\|_p := \|f\|_p$ ($\|.\|_p$ is well defined, because $\|f\|_p = \|g\|_p$ if $f \sim g$). When defined on $L^p(\Omega, \mathcal{A}, \mu)$, $\|.\|_p$ is indeed a norm, because $\|[f]\|_p = 0$ implies that $f(x) = 0$ almost everywhere, and therefore $[f] = [0]$. We conclude that, for every $1 \leq p \leq \infty$, $(L^p(\Omega, \mathcal{A}, \mu), \|.\|_p)$ is a normed vector space. As every norm, $\|.\|_p$ induces a metric on $L^p(\Omega, \mathcal{A}, \mu)$ (the metric is defined by $d(f, g) = \|f - g\|_p$), and thus a notion of convergence for sequences in $L^p(\Omega, \mathcal{A}, \mu)$.

**Theorem A.1.1.** *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, $1 \leq p \leq \infty$. Then $L^p(\Omega, \mathcal{A}, \mu)$, equipped with the norm $\|.\|_p$. is a Banach space, ie. it is a normed vector space, complete with respect to the metric induced by $\|.\|_p$. In other words, every Cauchy sequence on $L^p(\Omega, \mathcal{A}, \mu)$ converges.*

**Definition A.1.2** (Hilbert space)**.** *Let $\mathcal{H}$ be a vector space over $\mathbb{C}$, equipped with a scalar product $\langle \cdot, \cdot \rangle$ and let $\| \cdot \|$ be the norm induced by this scalar product. If $\mathcal{H}$, equipped with this norm, is complete, then the pair $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ is called a Hilbert space.*

A notable example of Hilbert space is the Lebesgue space $L^2(\Omega, \mathcal{A}, \mu)$. Indeed, we can define an inner product on $L^2(\Omega, \mathcal{A}, \mu)$. For $f, g \in L^2(\Omega, \mathcal{A}, \mu)$, we set

$$\langle f, g \rangle = \int \overline{f} g \, d\mu \tag{A.49}$$

It is easy to check that $\langle \cdot, \cdot \rangle$ is linear in its second argument, and antisymmetric (ie. $\langle g, f \rangle = \overline{\langle f, g \rangle}$). Moreover,

$$\langle f, f \rangle = \|f\|_2^2 \geq 0$$

Thus $\langle \cdot, \cdot \rangle$ is an inner product on $L^2(\Omega, \mathcal{A}, \mu)$ and it induces the norm $\| \cdot \|_2$. Hence, $L^2(\Omega, \mathcal{A}, \mu)$ is a Hilbert space. In particular, we have the Cauchy-Schwarz inequality

$$\left| \int \overline{f} g \, d\mu \right| = |\langle f, g \rangle| \leq \|f\|_2 \|g\|_2$$

for all $f, g \in L^2(\Omega, \mathcal{A}, d\mu)$.
The generalization of Cauchy-Schwarz inequality to $L^p$-spaces is called Hölder's inequality.

**Theorem A.1.3** (Hölder's inequality)**.** *Let $1 \leq p, p' \leq \infty$, with $1/p + 1/p' = 1$. For $f \in L^p(\Omega, \mathcal{A}, \mu), g \in L^{p'}(\Omega, \mathcal{A}, \mu)$, we have*

$$\left| \int \overline{f} g \, d\mu \right| \leq \int |f||g| d\mu \leq \|f\|_p \|g\|_{p'} \tag{A.50}$$

**The dual of $L^p(\Omega, \mathcal{A}, \mu)$.** For an arbitrary normed vector space $(X, \|.\|)$ over $\mathbb{C}$, a linear functional on $X$ is a linear map $L : X \to \mathbb{C}$. A linear functional $L$ is continuous if and only if it is bounded, ie. if there exists a constant $C > 0$ such that $|L(f)| \leq C\|f\|$ for all $f \in X$. We define the dual space of $X$ as

$$X^* = \{L : X \to \mathbb{C} : \ L \text{ is a continuous linear functional on } X\}$$

On $X^*$ we can naturally introduce a sum and a multiplication with complex numbers. Hence $X^*$ is a vector space. Since continuous functionals are bounded, we can also introduce a norm on $X^*$, by setting, for $L \in X^*$,

$$\|L\| = \sup_{f \in X : \|f\| \leq 1} |L(f)| = \sup_{f \in X : f \neq 0} \frac{|L(f)|}{\|f\|} \tag{A.51}$$

Equipped with this norm, $X^*$ is a normed vector space. In fact, $X^*$ is always complete (w.r.t. the norm (A.51), of course), and thus a Banach space.

In the following, we would like to characterize the dual space of $L^p(\Omega, \mathcal{A}, \mu)$. To this end, we observe that, choosing $1 \leq p' \leq \infty$ so that $1/p + 1/p' = 1$, for every $g \in L^{p'}(\Omega, \mathcal{A}, \mu)$, we can define a linear functional $L_g : L^p(\Omega, \mathcal{A}, \mu) \to \mathbb{C}$ by setting

$$L_g(f) = \int f g d\mu$$

Linearity of $L_g$ is clear, continuity follows from Hölder's inequality. For $1 \leq p < \infty$, it turns out that all linear functionals on $L^p(\Omega, \mathcal{A}, \mu)$ have this form.

**Theorem A.1.4.** *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, $1 \leq p < \infty$ and $1 < p' \leq \infty$ with $1/p + 1/p' = 1$. If $p = 1$ and $p' = \infty$, we make the additional assumption that the measure space is sigma-finite. The map $\phi : L^{p'}(\Omega, \mathcal{A}, \mu) \to L^p(\Omega, \mathcal{A}, \mu)^*$ defined by $\phi(g) = \phi_g : L^p(\Omega, \mathcal{A}, \mu) \to \mathbb{C}$, with*

$$\phi_g(f) = \int f g d\mu$$

*is an isometric isomorphism, meaning that it is linear, it preserves the norm, in the sense that $\|\phi_g\|_{L^p(\Omega,\mathcal{A},\mu)^*} = \|g\|_{L^{p'}}$, and it is a bijection.*

*Remark:* If $p = \infty$ and $p' = 1$, the map $\phi : L^1(\Omega, \mathcal{A}, \mu) \to L^\infty(\Omega, \mathcal{A}, \mu)^*$ is still well defined, linear, isometric (and therefore injective), but it is (in general) not surjective.

## A.2 Self-adjoint operators

On the Hilbert space $\mathcal{H}$ we define linear operators $A : \mathcal{H} \to \mathcal{H}$ as maps from the Hilbert space $\mathcal{H}$ to itself satisfying linearity, i.e.

$$A(\lambda f + \mu g) = \lambda A(f) + \mu A(g), \text{for all } f, g \in \mathcal{H}, \quad \forall\ \lambda, \mu \in \mathbb{R}$$

Such operators are called self-adjoint if

$$\langle f\ ,\ A\, g \rangle = \langle A\, f\ ,\ g \rangle \qquad \forall\, f, g \in \mathcal{H}.$$

An operator is called *bounded* if for all elements of the domain (in this case $\forall\ f \in \mathcal{H}$) there exists a positive constant $C$ such that

$$\|Af\| \leq C\|f\|, \tag{A.52}$$

where $\|\cdot\|$ is the norm induced by the inner product on $\mathcal{H}$. The operator norm of a bounded operator is defined as the minimal constant $C$ for which (A.52) holds true. Let $|||A|||$ denote the operator norm of the operator $A$, then the following characterization holds:

$$|||A||| = \sup_{f \in \mathcal{H}\ :\ \|f\| \leq 1} \frac{\|Af\|}{\|f\|}.$$

**Proposition A.2.1.** *For any bounded operator $A$, there is a unique bounded operator $A^*$, called the adjoint of $A$, such that*

$$\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle \qquad \forall \phi, \psi \in \mathcal{H}$$

The proof of the proposition replies on the celebrated Riesz Theorem:

**Theorem A.2.2** (Riesz's Theorem)**.** *If $\xi : \mathcal{H} \to \mathbb{C}$ is a bounded linear functional, then there exists a unique $\chi \in \mathcal{H}$ sich that $\xi(\psi) = \langle \chi, \psi \rangle$ for all $\psi \in \mathcal{H}$.*

*Proof of Proposition A.2.1.* For each fixed $\phi \in \mathcal{H}$ consider the map $\psi \mapsto \langle \phi, A\psi \rangle$ for all $\psi \in \mathcal{H}$. For each fixed $\phi \in \mathcal{H}$, the map is a linear functional on $\mathcal{H}$. Therefore, by Riesz's Theorem, there exists a unique $\chi \in \mathcal{H}$ such that $\langle \chi, \psi \rangle = \langle \phi, A\psi, \rangle$ and we use the notation $\chi = A^*\phi$. Boundedness and linearity follow from the boundedness of $A$ and by construction of the map. □

**Definition A.2.3.** *$A$ is an unbounded operator on $\mathcal{H}$ if it is not a bounded operator and it is a linear map from a dense subspace $\mathcal{D}(A) \subset \mathcal{H}$ into $\mathcal{H}$.*

**Definition A.2.4.** *Let $A$ be an unbounded operator on $\mathcal{H}$. $A^*$ is defined as follows:*

*i) $\phi \in \mathcal{H}$ belongs to $\mathcal{D}(A^*)$ if $\phi \mapsto \langle \phi, A\cdot \rangle$ defined on $\mathcal{H}$ is bounded;*

*ii) for each $\phi \in \mathcal{D}(A^*)$, $A^*\phi$ is the unique vector $\chi \in \mathcal{H}$ such that $\langle \chi, \psi \rangle = \langle \phi, A\psi \rangle$, for all $\psi \in \mathcal{D}(A)$.*

**Definition A.2.5.** *An unbounded operator $A$ on $\mathcal{H}$ is symmetric if $\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$ for all $\psi, \phi \in \mathcal{D}(A)$.*
*It is self-adjoint if $\mathcal{D}(A) = \mathcal{D}(A^*)$ and $A^*\phi = A\phi$ for all $\phi \in \mathcal{D}(A)$.*

## A.3 The Fourier Transform

For $f \in L^1(\mathbb{R}^d)$, we define the Fourier transform $\hat{f} : \mathbb{R}^d \to \mathbb{C}$ of $f$, setting

$$\hat{f}(k) = \frac{1}{(2\pi)^{d/2}} \int f(x) e^{-ik\cdot x} d\lambda_d(x), \tag{A.53}$$

where $\lambda_d$ is the Lebesgue measure in $\mathbb{R}^d$.
The Fourier transform has the following important properties.

- *Boundedness and continuity.* Let $f \in L^1(\mathbb{R}^d)$. Then $\hat{f} \in L^\infty(\mathbb{R}^d)$ with

  $$\|\hat{f}\|_\infty \leq (2\pi)^{-d/2} \|f\|_1$$

  Moreover, $\hat{f}$ is continuous.

- *Riemann-Lebesgue Lemma.* Let $f \in L^1(\mathbb{R}^d)$. Then $\hat{f}(k) \to 0$, as $|k| \to \infty$.

- *Fourier transform of convolutions.* For $f, g \in L^1(\mathbb{R}^d)$ we have (from Young's inequality) $f * g \in L^1(\mathbb{R}^d)$. Then

  $$\widehat{f * g}(k) = (2\pi)^{d/2} \hat{f}(k) \hat{g}(k)$$

- *Fourier transform of a Gaussian.* Let $f_\alpha(x) = e^{-\alpha x^2/2}$. Then

  $$\hat{f}_\alpha(k) = \alpha^{-d/2} e^{-k^2/2\alpha}$$

- *Derivatives and Fourier transform.* Let $f \in L^1(\mathbb{R}^d)$, and $g : \mathbb{R}^d \to \mathbb{C}^d$ be defined through $g(x) = -ixf(x)$. If $g$ is integrable, then $\hat{f} \in C^1(\mathbb{R}^d)$ with $\nabla \hat{f} = \hat{g}$.
- *Plancherel's identity.* Let $f \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$. Then $\hat{f} \in L^2(\mathbb{R}^d)$ and $\|\hat{f}\|_2 = \|f\|_2$.

Plancherel's identity can be used to extend the Fourier transform to $L^2$. For an arbitrary $f \in L^2(\mathbb{R}^d)$, we can find a sequence $f_j \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ with $f_j \to f$ in $L^2$. Since $f_j \in L^1(\mathbb{R}^d)$, we can define the Fourier transform $\hat{f}_j$. From Plancherel's identity, it follows that $\hat{f}_j \in L^2(\mathbb{R}^d)$, with $\|\hat{f}_j\|_2 = \|f_j\|_2$. Moreover

$$\|\hat{f}_j - \hat{f}_m\|_2 = \|\widehat{f_j - f_m}\|_2 = \|f_j - f_m\|_2 \to 0$$

as $j, m \to \infty$. We conclude that $\hat{f}_j$ is a Cauchy sequence in $L^2(\mathbb{R}^d)$ and thus it must converge. We can therefore define

$$\hat{f} = \lim_{j \to \infty} \hat{f}_j. \tag{A.54}$$

It is important to observe that $\hat{f}$ does not depend on the choice of the sequence $f_j \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$. The map $\hat{\cdot} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is clearly linear and isometric, i.e. $\|\hat{f}\|_2 = \|f\|_2$. It also preserves the inner product, i.e. $\langle \hat{f}; \hat{g} \rangle = \langle f; g \rangle$ for all $f, g \in L^2(\mathbb{R}^d)$. In fact, $\hat{\cdot} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is also invertible (the inverse is the map $\check{\cdot} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$, defined by $\check{f}(k) := \hat{f}(-k)$ for all $f \in L^2(\mathbb{R}^d)$). Thus, the Fourier transform $\hat{\cdot} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is a unitary map.

So far, we defined the Fourier transform as a linear map from $L^1(\mathbb{R}^d)$ to $L^\infty(\mathbb{R}^d)$ and as a linear map from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$. By interpolation, it can also be extended as a linear map from $L^p(\mathbb{R}^d)$ to $L^{p'}(\mathbb{R}^d)$, for all $1 < p < 2$, choosing $2 < p' < \infty$ so that $1/p + 1/p' = 1$. The extension is based on the Hausdorff-Young inequality (which replace the Plancherel's identity, for $p < 2$).

**Theorem A.3.1.** *Let $1 \leq p \leq 2$ and $2 \leq p' \leq \infty$ such that $1/p + 1/p' = 1$. Then there exists a constant $C > 0$ (depending on the dimension $n$ and on $p$) such that $\hat{f} \in L^{p'}(\mathbb{R}^n)$ and*

$$\|\hat{f}\|_{p'} \leq C \|f\|_p \tag{A.55}$$

*for any $f \in L^1(\mathbb{R}^d) \cap L^p(\mathbb{R}^d)$.*

## A.4 Distributions and Sobolev Spaces

**Definition and basic properties.** We start with the definition of the space of test functions.

**Definition A.4.1.** *Let $n \in \mathbb{N} \backslash \{0\}$ and $\Omega \subset \mathbb{R}^n$ be an open non-empty set ($\Omega = \mathbb{R}^n$ is allowed). We denote the space of test functions on $\Omega$ by $\mathcal{D}(\Omega)$. It consists of all functions in $C_c^\infty(\Omega)$ (the space of infinitely differentiable functions that are compactly supported inside $\Omega$), equipped with the following notion of convergence. A sequence $\phi_m \in C_c^\infty(\Omega)$ converges in $\mathcal{D}(\Omega)$ to $\phi \in C_c^\infty(\Omega)$ if and only if there exists a fixed compact set $K \subset \Omega$ such that supp $(\phi_m - \phi) \subset K$ for all $m \in \mathbb{N}$ and*

$$D^\alpha \phi_m \to D^\alpha \phi$$

*uniformly on $K$, for all multi-index $\alpha \in \mathbb{N}^n$. In other words,*

$$\sup_{x\in K}\left|\frac{\partial^{|\alpha|}\phi_m(x)}{\partial x_1^{\alpha_1}\dots\partial x_n^{\alpha_n}}-\frac{\partial^{|\alpha|}\phi(x)}{\partial x_1^{\alpha_1}\dots\partial x_n^{\alpha_n}}\right|\to 0$$

*as $m\to\infty$, for all $\alpha=(\alpha_1,\dots,\alpha_n)\in\mathbb{N}^n$ (with $|\alpha|=\alpha_1+\dots+\alpha_n$).*

Distributions are then continuous linear functionals on $\mathcal{D}(\Omega)$ (since the notion of convergence on $\mathcal{D}(\Omega)$ is very strong, it is very easy for a linear functional on $\mathcal{D}(\Omega)$ to be continuous).

**Definition A.4.2.** *A distribution $T$ is a continuous linear functional on the space of test functions $\mathcal{D}(\Omega)$. In other words, it is a map $T:\mathcal{D}(\Omega)\to\mathbb{C}$, with*

$$T(\phi_1+\lambda\phi_2)=T(\phi_1)+\lambda T(\phi_2)$$

*for all $\lambda\in\mathbb{C}$, $\phi_1,\phi_2\in\mathcal{D}(\Omega)$, such that $T(\phi_m)\to T(\phi)$ as $m\to\infty$, whenever $\phi_m\to\phi$ in $\mathcal{D}(\Omega)$. We denote by $\mathcal{D}'(\Omega)$ the space of distributions on $\Omega$. Observe that $\mathcal{D}'(\Omega)$ has the structure of a vector space (distributions can be summed and multiplied with scalars $\lambda\in\mathbb{C}$).*

An important observation is that every $L^p$-function defines a distribution. Since the behavior at infinity is not important, we define local $L^p$-spaces.

**Definition A.4.3.** *For $1\le p\le\infty$, we define the space of locally $p$-th power integrable functions*

$$L^p_{loc}(\Omega)=\{f:\Omega\to\mathbb{C}\text{ measurable such that }\|f\|_{L^p(K)}<\infty\text{ for all }K\subset\Omega\text{ compact}\}$$

*Notice that $L^p_{loc}(\Omega)$ is a vector space. In contrast with $L^p(\Omega)$, however, there is no natural norm on $L^p_{loc}(\Omega)$. Notice also that $L^q_{loc}(\Omega)\subset L^p_{loc}(\Omega)$ if $1\le p\le q\le\infty$. In particular, $L^1_{loc}(\Omega)\supset L^p_{loc}(\Omega)\supset L^p(\Omega)$ for all $1\le p\le\infty$.*

Every locally integrable function defines a distribution.

**Lemma A.4.4.** *Let $\Omega\subset\mathbb{R}^n$ open, non-empty, $f\in L^1_{loc}(\Omega)$. We define $T_f:\mathcal{D}(\Omega)\to\mathbb{C}$ setting*

$$T_f(\phi)=\int_\Omega f\phi\,d\lambda_n(x) \tag{A.56}$$

*for all $\phi\in\mathcal{D}(\Omega)$. Then $T_f\in\mathcal{D}'(\Omega)$ is a distribution (it is the distribution associated with $f$).*

While every locally integrable function $f\in L^1_{\text{loc}}(\Omega)$ defines a distribution $T_f\in\mathcal{D}'(\Omega)$, not every distribution in $\mathcal{D}'(\Omega)$ has the form $T_f$ for an $f\in L^1_{\text{loc}}(\Omega)$. An example of a distribution which is not associated with a locally integrable function is the Dirac delta-distribution

$$\delta_x(\phi)=\phi(x) \tag{A.57}$$

for all $\phi\in\mathcal{D}(\Omega)$ and for a $x\in\Omega$.

**Distributional derivatives and Sobolev spaces.** The derivative of a distribution is defined as follows.

**Definition A.4.5.** *Let $\Omega \subset \mathbb{R}^n$ be open and non-empty, $T \in \mathcal{D}'(\Omega)$ a distribution. For a multi-index $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$, we define $D^\alpha T \in \mathcal{D}'(\Omega)$ through*

$$D^\alpha T(\phi) = (-1)^{|\alpha|} T(D^\alpha \phi) \tag{A.58}$$

*with $|\alpha| = \alpha_1 + \cdots + \alpha_n$.*

*Remark:* Let $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$ be a multi-index and $f \in C^{|\alpha|}(\Omega)$. In this case, we have $D^\alpha T_f = T_{D^\alpha f}$. In other words, if we identify functions with the corresponding distributions, classical derivatives coincide, when they exist, with distributional derivatives. But, of course, distributional derivatives are much more general, since they can be applied to arbitrary locally integrable functions (for which classical derivatives do not need to exist) and, even more generally, to arbitrary distributions.

We can now define the Sobolev space $W^{m,p}(\Omega)$ as the space of all functions $f \in L^p(\Omega)$ whose distributional derivatives of order up to $m$ (defined through the distribution $T_f$ associated with $f$) are again functions in $L^p(\Omega)$.

**Definition A.4.6.** *For $\Omega \subset \mathbb{R}^n$ open, non-empty, $m \in \mathbb{N}$ and $1 \leq p \leq \infty$, we define*

$$W^{m,p}(\Omega) = \{f \in L^p(\Omega) : \forall\, \alpha \in \mathbb{N}^n \text{ with } |\alpha| \leq m \text{ there is } g_\alpha \in L^p(\Omega) \text{ with } D^\alpha T_f = T_{g_\alpha}\}$$

*For $f \in W^{m,p}(\Omega)$ and $\alpha \in \mathbb{N}^n$ with $|\alpha| \leq m$, we define $D^\alpha f = g_\alpha \in L^p(\Omega)$ (the functions $D^\alpha f$ are known as the distributional or weak derivatives of $f$). For $1 \leq p < \infty$, we define*

$$\|f\|_{W^{m,p}} = \left[ \sum_{\alpha \in \mathbb{N}^n : |\alpha| \leq m} \|D^\alpha f\|_p^p \right]^{1/p}$$

*For $p = \infty$, we set*

$$\|f\|_{W^{m,\infty}} = \sum_{|\alpha| \leq m} \|D^\alpha f\|_\infty.$$

*Then $\|.\|_{W^{m,p}}$ is a norm on $W^{m,p}(\Omega)$ and $(W^{m,p}(\Omega), \|.\|_{W^{m,p}})$ is a complete Banach space.*

An important property of functions in the Sobolev space $W^{m,p}(\Omega)$, for $1 \leq p < \infty$, is the fact that they can be approximated by sequences of smooth functions. This is known as the Meyers-Serrin theorem.

**Theorem A.4.7.** *Let $m \in \mathbb{N}$, $1 \leq p < \infty$, $\Omega \subset \mathbb{R}^n$ open, non-empty. Let $f \in W^{m,p}(\Omega)$. Then there exists a sequence $f_j \in C^\infty(\Omega) \cap W^{m,p}(\Omega)$ such that*

$$\|f - f_j\|_{W^{m,p}(\Omega)} \to 0$$

*as $j \to \infty$. If $\Omega = \mathbb{R}^n$, the sequence $f_j$ can be chosen in $C_c^\infty(\mathbb{R}^n)$ (ie. to have compact support).*

*Remark.* If $\Omega \subset \mathbb{R}^n$ has a boundary and $m \in \mathbb{N}\backslash\{0\}$, $C_c^\infty(\Omega)$ is not dense in $W^{m,p}(\Omega)$. The completion of $C_c^\infty(\Omega)$ with respect to the $W^{m,p}(\Omega)$ norm is a subspace of $W^{m,p}(\Omega)$, typically denoted by $W_0^{m,p}(\Omega)$, which is used to solve differential equations with Dirichlet boundary conditions.

**The Hilbert spaces $H^m(\Omega)$.** Let $\Omega \subset \mathbb{R}^n$ open and non-empty, $m \in \mathbb{N}$. We will use the notation $H^m(\Omega)$ for the space $W^{m,2}(\Omega)$. For $f, g \in H^m(\Omega)$, we define the inner product

$$\langle f; g\rangle_{H^m} = \sum_{\alpha\in\mathbb{N}^n:|\alpha|\leq m} \langle D^\alpha f; D^\alpha g\rangle_2$$

where $\langle .; .\rangle_2$ denotes the usual inner product on $L^2(\Omega)$. Clearly,

$$\|f\|^2_{W^{m,2}} \equiv \|f\|^2_{H^m} = \langle f; f\rangle_{H^m}.$$

Thus, $(H^m(\Omega), \langle .; .\rangle_{H^m})$ is a Hilbert space.

For $\Omega = \mathbb{R}^n$, there is a useful characterisaztion of $H^m(\Omega)$ in terms of Fourier transform.

**Theorem A.4.8.** *Let $f \in L^2(\mathbb{R}^n)$, and $\hat{f} \in L^2(\mathbb{R}^n)$ be its Fourier transform. Then $f \in H^m(\mathbb{R}^n)$ if and only if the function $k \to |k|^m \hat{f}(k)$ is in $L^2(\mathbb{R}^n)$. In this case, the distributional derivatives of $f$ satisfy $\widehat{D^\alpha f}(k) = i^{|\alpha|}k^\alpha \hat{f}(k)$ for all $\alpha \in \mathbb{N}^n$ with $|\alpha| \leq m$ and therefore*

$$\|f\|^2_{H^m} = \sum_{\alpha\in\mathbb{N}^n:|\alpha|\leq m} \int_{\mathbb{R}^n} |k_1|^{2\alpha_1}|k_2|^{2\alpha_2}\dots|k_n|^{2\alpha_n}\,|\hat{f}(k)|^2 dk$$

**Green's functions of the Laplacian.** Let $G_2(x) = (2\pi)^{-1}\log|x-y|$ and, for $n \in \mathbb{N}$, $n \geq 3$,

$$G_n(x) = \frac{1}{(n-2)|S^{n-1}|}\frac{1}{|x|^{n-2}}$$

where $|S^{n-1}| = 2\pi^{n/2}/\Gamma(n/2)$ is the measure of the $(n-1)$-dimensional sphere with radius one. Then, we have, in the sense of distributions,

$$-\Delta G_n = \delta \tag{A.59}$$

where $\delta \in \mathcal{D}'(\mathbb{R}^n)$ is defined through $\delta(\phi) = \phi(0)$. Thus, if $f \in L^1_{\text{loc}}(\mathbb{R}^n)$ such that $y \to G_n(x-y)f(y)$ is integrable, for almost every $x \in \mathbb{R}^n$, then the function $u = G_n * f \in L^1_{\text{loc}}(\mathbb{R}^n)$ solves the Poisson equation $-\Delta u = f$, in the sense of distributions.

## A.5 Sobolev Inequalities and Sobolev Embeddings

**Sobolev inequalities for gradients.** We begin with the standard Sobolev inequality for functions in $H^1(\mathbb{R}^n)$, $n \geq 3$.

**Theorem A.5.1.** *Let $n \in \mathbb{N}$, $n \geq 3$. Let $f \in H^1(\mathbb{R}^n)$. Then $f \in L^q(\mathbb{R}^n)$, for $q = 2n/(n-2)$. Moreover, there exists a constant $C_n$ (depending only on the dimension $n$) such that*

$$\|f\|_q \leq C_n\|\nabla f\|_2 \tag{A.60}$$

*for all $f \in H^1(\mathbb{R}^n)$.*

In dimensions $n = 1, 2$, we cannot bound high $L^q$ norms just with the $L^2$ norm of $\nabla f$, we also need the $L^2$ norm of $f$.

**Theorem A.5.2.** *One-dimension: There exists a constant $C > 0$ such that*

$$\|f\|_q \leq C\|f\|_{H^1}$$

*for all $f \in H^1(\mathbb{R})$ and all $2 \leq q \leq \infty$. Moreover, every $f \in H^1(\mathbb{R})$ has a representative satisfying*

$$|f(x) - f(y)| \leq \|\partial f\|_2 |x - y|^{1/2}$$

*for all $x, y \in \mathbb{R}$. In other words, $H^1$-functions in one-dimension are automatically Hölder continuous with exponent $\alpha = 1/2$.*

*Two-dimensions: For every $2 \leq q < \infty$ there exists $C > 0$ such that*

$$\|f\|_q \leq C\|f\|_{H^1}$$

*for all $f \in H^1(\mathbb{R}^2)$.*

*Remark:* in two dimensions, the $L^\infty$-norm cannot be bounded by the $H^1$-norm.

**Compact Sobolev embedding**. The Sobolev inequality implies that the unit ball in $H^1(\mathbb{R}^n)$ is a subset of $L^q(\mathbb{R}^n)$, if $q \leq 2n/(n-2)$ (or if $q < \infty$ in two dimensions, $q \leq \infty$ in one dimension). When restricting on sets with finite measure, it turns out that the unit ball of $H^1$ is sequentially compact subset of $L^q$. This follows from the following theorem.

**Theorem A.5.3.** *Let $\{f_j\}_{j\in\mathbb{N}}$ be a weakly convergent sequence in $H^1(\mathbb{R}^n)$, let $f$ denote its weak limit. Let moreover $A \subset \mathbb{R}^n$ be a set of finite measure and $\chi_A$ the corresponding characteristic function. Then $\chi_A f_j \to \chi_A f$ strongly in $L^q(\mathbb{R}^n)$, for all $1 \leq q < 2n/(n-2)$, if $n \geq 3$, and for all $1 \leq q < \infty$, if $n = 1, 2$. For $n = 1$, the convergence is pointwise and uniform on every compact subset of $\mathbb{R}$.*

**General Sobolev inequalities and embedding theorems.** Sobolev inequalities can be extended to domains with the cone property, defined as follows.

**Definition A.5.4.** *For $r > 0$ and $\theta \in [0; 2\pi]$, let*

$$K_{r,\theta} := \{x \in \mathbb{R}^n : x \neq 0, 0 < x_n < |x| \cos\theta\} \cap B_r(0)$$

*denote a finite cone of angle $\theta$ and length $r$. We say that an open domain $\Omega \subset \mathbb{R}^n$ has the cone property if there exists $r, \theta$ such that, for all $x \in \Omega$ there is a finite cone $K_x$ congruent to $K_{r,\theta}$ which is contained in $\Omega$ and has vertex $x$.*

We state now the general form of Sobolev inequality.

**Theorem A.5.5.** *Let $\Omega \subset \mathbb{R}^n$ be an open set, with the cone property for some $r, \theta$. Let $1 \leq p \leq q \leq \infty$, $m, k \in \mathbb{N}$, with $m \geq 1$ and $k \leq m$. Then there exists a constant $C > 0$ (depending on $m, k, q, p, \theta, r$) such that, for all $f \in W^{m,p}(\Omega)$, we have*

*i) If $kp < n$,*

$$\|f\|_{W^{m-k,q}(\Omega)} \leq C\|f\|_{W^{m,p}(\Omega)}$$

*for all $p \leq q \leq np/(n-kp)$.*

*ii) If $kp = n$,*

$$\|f\|_{W^{m-k,q}(\Omega)} \leq C\|f\|_{W^{m,p}(\Omega)}$$

*for all $p \leq q < \infty$.*

*iii) If $kp > n$,*

$$\|f\|_{W^{m-k,q}(\Omega)} \leq C\|f\|_{W^{m,p}(\Omega)}$$

*for all $p \leq q \leq \infty$. In particular,*

$$\max_{0\leq|\alpha|\leq m-k} \sup_{x\in\Omega} |D^\alpha f(x)| \leq C\|f\|_{W^{m,p}(\Omega)}$$

The next theorem, known as the Rellich-Kondrachov theorem, provides the general statement for compact Sobolev embeddings.

**Theorem A.5.6.** *Let $\Omega \subset \mathbb{R}^n$ be an open set, with the cone property for some $r, \theta$. Let $1 \leq p \leq q \leq \infty$, $m, k \in \mathbb{N}$, with $m \geq 1$ and $k \leq m$. Let $f \in W^{m,p}(\Omega)$ and $\{f_j\}_{j\in\mathbb{N}}$ be a sequence in $W^{m,p}(\Omega)$ with $f_j \rightharpoonup f$ weakly in $W^{m,p}(\Omega)$ (meaning that $D^\alpha f_j \rightharpoonup D^\alpha f$ weakly in $L^p(\Omega)$, for all multiindex $\alpha \in \mathbb{N}^n$ with $0 \leq |\alpha| \leq m$). Let $\omega \subset \Omega$ be open and bounded (in particular, we can take $\omega = \Omega$, if $\Omega \subset \mathbb{R}^3$ is bounded). Then, we have*

*i) If $kp < n$, $1 \leq q < np/(n-kp)$, then $\|f_j - f\|_{W^{m-k,q}(\omega)} \to 0$, as $j \to \infty$.*

*ii) If $kp = n$, $1 \leq q < \infty$, then $\|f_j - f\|_{W^{m-k,q}(\omega)} \to 0$, as $j \to \infty$.*

*iii) If $kp > n$, $1 \leq q \leq \infty$, then $\|f_j - f\|_{W^{m-k,q}(\omega)} \to 0$, as $j \to \infty$. In particular, taking $q = \infty$, we conclude that*

$$\max_{0\leq|\alpha|\leq m-k} \sup_{x\in\omega} |D^\alpha f_j(x) - D^\alpha f(x)| \to 0$$

*as $j \to \infty$.*

**Poincaré inequality.** Finally, let us also mention a useful variant of the Sobolev inequality, known as the Poincaré inequality, which allows us to bound fluctuations of functions in Sobolev spaces.

**Theorem A.5.7.** *Let $\Omega \subset \mathbb{R}^n$ be a bounded, connected, open set with the cone property for some $r, \theta$. Let $1 \leq p < \infty$, and let $g \in L^{p'}(\Omega)$ with $\int g d\lambda_n = 1$. Then there exists a constant $C = C(\Omega, g, p, q)$ such that*

$$\left\| f - \int_\Omega fg \, d\lambda_n \right\|_{L^q(\Omega)} \leq C\|\nabla f\|_{L^p(\Omega)}$$

*for all $f \in W^{1,p}(\Omega)$ and all $1 \leq q < pn/(n-p)$ if $p < n$, all $1 \leq q < \infty$ if $p = n$, and all $1 \leq q \leq \infty$ if $p > n$.*