

METHODS OF MODERN MATHEMATICAL PHYSICS
UNCERTAINTY AND EXCLUSION PRINCIPLES IN QUANTUM MECHANICS

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ABSTRACT. These are lecture notes for a master-level course with the primary aim of proving the stability of matter from first principles using modern mathematical methods in many-body quantum mechanics. General quantitative formulations of the uncertainty and the exclusion principles of quantum mechanics are introduced, such as the Hardy, Sobolev and Poincaré functional inequalities as well as the powerful Lieb–Thirring inequality that combines these two principles. The notes are aimed to be both fairly self-contained and at the same time complementary to existing literature, also covering recent developments to prove Lieb–Thirring inequalities and stability from general, weaker formulations of the exclusion principle.

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1. INTRODUCTION

Most of us take the stability of the world around us — as observed to consist of atoms, molecules, and even larger lumps of matter such as rocks, biological beings and entire planets — for granted every day. There is nothing strange about it. However, proving mathematically from first principles of mechanics that this is indeed so turns out to be surprisingly challenging and subtle. It was considered to be one of the great triumphs of mathematical physics when this problem was solved, first by Dyson and Lenard in 1967 [DL67], then in a better understood approach by Lieb and Thirring in 1975 [LT75]. Subsequently further details have been worked out over several decades by numerous other mathematicians and physicists [LS10]. Its resolution turns out to rest fundamentally on the two basic principles of quantum mechanics: the **uncertainty principle** and the **(Pauli) exclusion principle**. Namely, without these two concepts, i.e. relying strictly on the (indeed very well-founded) framework for mechanics which was available at the end of the 19th century and nowadays called classical mechanics, matter turns out to be *unstable* because the orbit of an electron around the nucleus of an atom can be made arbitrarily small and the electron may thus crash into the nucleus. Quantum mechanics came in to resolve this puzzle by introducing the idea that electron orbits are quantized into a discrete set of spatial probability distributions, with a smallest approximate radius called the Bohr radius. This prevents the electron from falling further into the attractive and infinitely deep potential well caused by the nucleus, and seemingly leads to the stability of matter. Indeed, most physicists are content with this answer even today, and the typical quantum mechanics textbook digs no further into the issue. However, a more careful mathematical analysis of the usual argument invoked (known as Heisenberg’s formulation of the uncertainty principle) leads to the realization that it remains *insufficient* to rigorously prove stability. Stronger formulations of

the uncertainty principle, such as the functional inequalities known as Hardy's or Sobolev's inequality, may instead be used to prove that an atom is indeed stable.

This is not the end of the story, however, because evidently the world consists of many more particles than just one single atom, with a mix of attractive and repulsive electromagnetic forces between them, and it turns out to be a very subtle issue to understand why in fact taking two similar lumps of matter and putting them together produces just twice the amount of matter when it comes to volume and energy, and why not some new state forms which is more favorable energetically and takes much less space. Here the Pauli exclusion principle comes into play, which tells us that particles such as electrons (and generally known as fermions) cannot all occupy the same quantum state, but must rather move into different configurations, such as different atom orbitals. This is what gives rise to the periodic table of the elements along with their chemical properties, and effectively produces larger and larger atoms and molecules, and in general, matter whose energy and volume scales *linearly* with the number of particles. The effect makes its presence all the way up to the size of stars, and explains for example why certain astronomical objects known as white dwarfs do not collapse under their own extreme gravitation to form black holes.

The story of the problem of stability of matter, from the invention of quantum mechanics to present times, is told as it should — in the rigorous language of mathematics — in the one textbook on the subject, namely [LS10], to which we refer the reader for a more complete account of its background and subsequent developments in various directions. The aim of these lecture notes is to provide an as concise as possible, and at the same time rigorous and self-contained, path to stability via a powerful functional inequality introduced by Lieb and Thirring which elegantly combines the uncertainty and exclusion principles. However, we will in contrast to [LS10] take a recently developed route to proving this inequality, which actually lies closer in spirit to the original Dyson–Lenard approach. In particular, the way we incorporate the exclusion principle will make transparent its role in the proof of stability as an effective repulsion between particles, and furthermore clarifies that it also extends to other particles than those obeying the usual Pauli principle, as long as they experience a strong enough repulsive interaction. For completeness and in order to further complement [LS10], these notes also contain some mathematical preliminaries and some background material on classical and quantum mechanics aimed for mathematicians, including a general discussion on identical particles and quantum statistics. In parallel with our general treatment of exclusion principles we also discuss a wide variety of formulations of the uncertainty principle, both global and local with respect to the configuration space, though we typically focus on their conceptual content rather than the most precise formulation or the optimal constants.

This version of the lecture notes, dated May 2018, still lacks some of the intended topics and corrections, however they will hopefully anyway find use in a wider audience.

A brief note concerning the notation: In the many-body context we usually write $x \in \mathbb{R}$ for scalars, $\mathbf{x} \in \mathbb{R}^d$ for one-body vectors, and $\mathbf{x} \in \mathbb{R}^n$ for general or many-body vectors, such as $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) \in (\mathbb{R}^d)^N = \mathbb{R}^{dN}$. The letter C will generally denote a constant whose exact value is unimportant and which may vary from one expression to another. Remarks with * signify that some more background (in math or physics) is required.

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2. SOME PRELIMINARIES AND NOTATION

We assume that the reader is familiar with basic notions in real analysis and has already encountered for example Hilbert spaces, Lebesgue integrals, as well as Fourier transforms. However, for convenience and for setting our notation we give here a very brief overview of these and a few other important concepts. See [LL01, RS72, RS75, Tes14, Thi02] for more.

2.1. Hilbert spaces. We let V denote a vector space of arbitrary dimension over the scalars $\mathbb{F} = \mathbb{R}$ or \mathbb{C} , and $z \mapsto \bar{z}$ complex conjugation.

Definition 2.1. A **sesquilinear form** on V is a map $V \times V \rightarrow \mathbb{F}$, $(u, v) \mapsto \langle u, v \rangle$ such that for all $\alpha, \beta \in \mathbb{F}$, $u, v, w \in V$:

- (i) $\langle u, \alpha v + \beta w \rangle = \alpha \langle u, v \rangle + \beta \langle u, w \rangle$ (linear in the *second*⁽¹⁾ argument),
- (ii) $\langle \alpha u + \beta v, w \rangle = \bar{\alpha} \langle u, w \rangle + \bar{\beta} \langle v, w \rangle$ (conjugate linear in the *first* argument).

A **hermitian form** on V is a sesquilinear form $\langle \cdot, \cdot \rangle$ satisfying, in addition:

- (iii) $\langle u, v \rangle = \overline{\langle v, u \rangle}$ (symmetry).

An **inner product** or **scalar product** on V is a hermitian form $\langle \cdot, \cdot \rangle$ satisfying, in addition:

- (iv) $\langle v, v \rangle > 0$ for $v \neq 0$ (positive definite).

A (sesqui-) **quadratic form** on V is a map $q: V \rightarrow \mathbb{F}$ such that for $\alpha \in \mathbb{F}$, $u, v \in V$:

- (i) $q(\alpha v) = \bar{\alpha} \alpha q(v)$ (scaling quadratically),
- (ii) $\langle u, v \rangle_q := \frac{1}{4}(q(u+v) - q(u-v) + iq(u-iv) - iq(u+iv))$ is sesquilinear in u, v .

A **norm** on V is a map $V \rightarrow \mathbb{R}_+ := [0, \infty)$, $v \mapsto \|v\|$, such that for all $\alpha \in \mathbb{F}$, $u, v \in V$:

- (i) $\|\alpha v\| = |\alpha| \|v\|$ (scaling linearly),
- (ii) $\|u+v\| \leq \|u\| + \|v\|$ (triangle inequality),
- (iii) $\|v\| = 0$ if and only if $v = 0$ (positive definite).

The pair $(V, \|\cdot\|)$ is called a **normed linear space**, the pair (V, q) a (sesqui-) **quadratic space**, and the pair $(V, \langle \cdot, \cdot \rangle)$ an **inner product space** or a **pre-Hilbert space**.

Example 2.2. The space \mathbb{C}^n of n -tuples $z = (z_1, \dots, z_n)$ with the standard inner product $\langle z, w \rangle = \sum_{j=1}^n \bar{z}_j w_j$ and norm $\|z\| = \sqrt{\langle z, z \rangle}$ is a normed, quadratic and pre-Hilbert space.

Example 2.3. Any normed linear space $(V, \|\cdot\|)$ satisfying the **parallelogram identity**

$$\|u+v\|^2 + \|u-v\|^2 = 2\|u\|^2 + 2\|v\|^2$$

is a quadratic space with $q(v) := \|v\|^2$, and an inner product space with

$$\langle u, v \rangle := \langle u, v \rangle_q = \frac{1}{4} \left(\|u+v\|^2 - \|u-v\|^2 + i\|u-iv\|^2 - i\|u+iv\|^2 \right)$$

(this nontrivial implication is known as the Jordan–von Neumann theorem). Conversely, any inner product space is also a normed space, as follows:

Proposition 2.4 (Cauchy–Schwarz inequality). *Let V be an inner product space. Then for every $u, v \in V$ we have*

$$|\langle u, v \rangle| \leq \|u\| \|v\| \tag{2.1}$$

with equality iff u and v are parallel.

⁽¹⁾Note that this convention varies in the literature; the one here is used in almost every physics text.

Because of the Cauchy-Schwarz inequality, the square root of the induced quadratic form $\|u\| := \sqrt{\langle u, u \rangle}$ satisfies the triangle inequality, by means of

$$\|u + v\|^2 = \|u\|^2 + 2 \operatorname{Re} \langle u, v \rangle + \|v\|^2 \leq (\|u\| + \|v\|)^2,$$

and hence becomes a norm on V . The norm induces a metric $d(u, v) := \|u - v\|$ and therefore a topology on V , with the open sets generated by balls defined using the metric,

$$B_r(x) := \{u \in V : d(x, u) < r\}.$$

Recall that a **Cauchy sequence** is a sequence $(v_n)_{n=1}^\infty \subset V$ such that

$$\forall \varepsilon > 0 \exists N \in \mathbb{N} : n, m > N \Rightarrow \|v_n - v_m\| < \varepsilon,$$

and a topological space is called **complete** if every Cauchy sequence converges. Also recall that a topological space is called **separable** if it contains a countable dense subset.

Definition 2.5. A complete normed linear space is called a **Banach space**. A complete inner product (i.e. pre-Hilbert) space is called a **Hilbert space**.

Lemma 2.6 (Riesz lemma; see e.g. [Tes14, Theorem 1.8]). *Suppose $\ell: V \rightarrow \mathbb{F}$ is a bounded linear functional on a Hilbert space V . Then there is a unique vector $u \in V$ s.t. $\ell(v) = \langle u, v \rangle$ for all $v \in V$.*

Exercise 2.1. *Prove (2.1) and Proposition 2.4, for example by considering the expression $\langle u - \alpha v, u - \alpha v \rangle$ with $\alpha = \langle v, u \rangle / \langle v, v \rangle$.*

Exercise 2.2. *Let V be a vector space, $s(u, v)$ a sesquilinear form on V , and $q(v) = s(v, v)$ the associated quadratic form. Prove that it satisfies the parallelogram identity*

$$q(u + v) + q(u - v) = 2q(u) + 2q(v)$$

*and the **polarization identity** $s(u, v) = \langle u, v \rangle_q$ for all $u, v \in V$. Show that $s(u, v)$ is hermitian if and only if q is real-valued, i.e. $q: V \rightarrow \mathbb{R}$, and that if q is non-negative, i.e. $q: V \rightarrow \mathbb{R}_+$, then it also satisfies the Cauchy-Schwarz inequality $|s(u, v)| \leq q(u)^{1/2} q(v)^{1/2}$.*

Exercise 2.3. *Let V be an inner product space and $\{u_j\}_{j=1}^n$ an **orthonormal** set in V , i.e. $\langle u_j, u_k \rangle = \delta_{jk}$. Prove **Bessel's inequality***

$$\sum_{j=1}^n |\langle u_j, v \rangle|^2 \leq \|v\|^2 \tag{2.2}$$

for all $v \in V$, with equality iff $v \in \operatorname{Span}\{u_j\}_{j=1}^n$.

2.2. Lebesgue spaces. The typical example of a Hilbert space encountered in quantum mechanics is either the finite-dimensional space \mathbb{C}^n , or the infinite-dimensional Lebesgue space of square-integrable functions $L^2(\Omega)$. Recall that for $\Omega \subseteq \mathbb{R}^n$ (which could be replaced by some measure space (X, μ) in general) and for a measurable function $f: \Omega \rightarrow \mathbb{F}$, we define the **L^p -norms** as

$$\|f\|_{L^p(\Omega; \mathbb{F})} := \left(\int_{\Omega} |f(x)|^p dx \right)^{1/p}, \quad 1 \leq p < \infty,$$

and

$$\|f\|_{L^\infty(\Omega; \mathbb{F})} := \operatorname{ess\,sup}_{x \in \Omega} |f(x)| := \inf \{K \in [0, \infty] : |f(x)| \leq K \text{ for a.e. } x \in \Omega\}.$$

Then the **Lebesgue spaces** are defined as

$$L^p(\Omega; \mathbb{F}) := \{f: \Omega \rightarrow \mathbb{F} : f \text{ is measurable and } \|f\|_{L^p(\Omega; \mathbb{F})} < \infty\}.$$

In the above $(\mathbb{F}, |\cdot|)$ can be taken to be any finite-dimensional normed space (algebra), however the typical case is $\mathbb{F} = \mathbb{C}$ for which we simply write $L^p(\Omega) := L^p(\Omega; \mathbb{C})$. If the domain Ω (or space (X, μ)) is also understood from context we could write simply $\|f\|_{L^p} := \|f\|_{L^p(\Omega)}$. We follow the standard convention that we identify two functions $f = g$ iff $f(x) = g(x)$ for a.e. $x \in \Omega$. It is a classical fact that $L^p(\Omega)$ forms a Banach space for any $p \in [1, \infty]$ and that $L^2(\Omega)$ is a separable Hilbert space with the standard inner product

$$\langle f, g \rangle := \int_{\Omega} \overline{f(x)} g(x) dx.$$

Proposition 2.7 (Hölder's inequality). *Let $1 \leq p, q, r \leq \infty$. For $L^p = L^p(\Omega; \mathbb{F})$ we then have⁽²⁾*

$$\|fg\|_{L^r} \leq \|f\|_{L^p} \|g\|_{L^q} \quad \text{for } \frac{1}{r} = \frac{1}{p} + \frac{1}{q}, \quad (2.3)$$

and for all $f \in L^p, g \in L^q$. In particular, with $p = q = 2$ and $r = 1$,

$$\|fg\|_{L^1} \leq \|f\|_{L^2} \|g\|_{L^2}$$

is the Cauchy-Schwarz inequality in L^2 . Moreover, if $p, q \in (1, \infty)$ then equality holds in (2.3) if and only if $|f|^p$ and $|g|^q$ are linearly dependent in L^1 .

There is a trick to remember the precise form of, or to check the validity of, inequalities or identities of the type (2.3). Namely, first note how it depends upon rescaling f or g with a positive number $\lambda > 0$, i.e. linearly on both sides of the inequality, since by the property of the norms $\|\lambda f\|_{L^p} = \lambda \|f\|_{L^p}$. Secondly, one should note how the expressions behave upon rescaling the argument of the functions f and g by a number $\mu > 0$, i.e. $f_{\mu}(x) := f(x/\mu)$,

$$\|f_{\mu}\|_{L^p} = \left(\int_{\Omega} |f(x/\mu)|^p dx \right)^{1/p} = \mu^{n/p} \|f\|_{L^p},$$

if $\Omega = \mu\Omega = \mathbb{R}^n$. Also in the case that $\Omega \subsetneq \mathbb{R}^n$ one may note that if f is dimensionless then the norm $\|f_{\mu}\|_{L^p}$ has the dimension of a volume in \mathbb{R}^n to the power $1/p$, i.e. n/p . We then find that the l.h.s. of (2.3) scales as $\mu^{n/r}$, but also the r.h.s. scales as $\mu^{n/p} \mu^{n/q} = \mu^{n/r}$. These two scaling principles must always be obeyed and can be used to check similar expressions.

An application of the Hölder inequality (2.3) proves the triangle inequality on L^p :

Proposition 2.8 (Minkowski's inequality). *Let $1 \leq p \leq \infty$. Then*

$$\|f + g\|_{L^p} \leq \|f\|_{L^p} + \|g\|_{L^p},$$

for all $f, g \in L^p$.

In the case that Ω is noncompact it is useful to define, given any function space $\mathcal{F}(\Omega; \mathbb{F})$ (such as $\mathcal{F} = L^p$), the *local* function space

$$\mathcal{F}_{\text{loc}}(\Omega; \mathbb{F}) := \{f: \Omega \rightarrow \mathbb{F} : \varphi f \in \mathcal{F}(\Omega; \mathbb{F}) \text{ for any } \varphi \in C_c^{\infty}(\Omega; \mathbb{F})\},$$

where $C_c^{\infty}(\Omega; \mathbb{F})$ denotes the space of smooth functions with compact support on Ω° .

⁽²⁾We use the convention $1/\infty = 0$.

Exercise 2.4. Prove Hölder's inequality, for example by

1. first reducing (2.3) to the case $\|fg\|_1 \leq \|f\|_p \|g\|_q$, $1 = 1/p + 1/q$, i.e. $r = 1$,
2. proving **Young's inequality**

$$ab \leq \frac{a^p}{p} + \frac{b^q}{q} \quad (2.4)$$

for such p, q and $a, b \geq 0$, with equality iff $a^p = b^q$,

3. using this to prove Hölder's inequality with $r = 1$ by first normalizing f and g .

Exercise 2.5. Prove Minkowski's inequality, f.ex. by writing $|f + g|^p = |f + g| |f + g|^{p-1}$ and then using the triangle and Hölder inequalities.

2.2.1. *Convergence properties.* One has the following extremely useful convergence properties of the Lebesgue integral:

Theorem 2.9. Let (X, μ) be a measure space with positive measure μ , and let $(f_n)_{n=1}^\infty$ be a sequence of measurable functions in $L^1(X, d\mu)$ that converges pointwise a.e. on X to a function f (it may then be redefined on a set of measure zero so that it too is measurable).

(i) **Lebesgue monotone convergence theorem.**

Suppose that $0 \leq f_n(x) \leq f_{n+1}(x)$ for a.e. $x \in X$. Then $\lim_{n \rightarrow \infty} \int_X f_n d\mu = \int_X f d\mu$ (which could be finite or infinite).

(ii) **Lebesgue dominated convergence theorem.**

Suppose that there exists $F \in L^1(X, d\mu)$ such that $|f_n(x)| \leq |F(x)|$ for a.e. $x \in X$. Then $f \in L^1(X, d\mu)$ and $\lim_{n \rightarrow \infty} \int_X |f_n - f| d\mu = 0$.

(iii) **Fubini's theorem.**

Suppose that $X = X_1 \times X_2$, where (X_j, μ_j) , $j = 1, 2$ are two σ -finite measure spaces, and that f is a measurable function on X . If $f \geq 0$ then the following three integrals are equal:

$$\begin{aligned} & \int_{X_1 \times X_2} f(x, y) (\mu_1 \times \mu_2)(dx dy), \\ & \int_{X_1} \left(\int_{X_2} f(x, y) \mu_2(dy) \right) \mu_1(dx), \\ & \int_{X_2} \left(\int_{X_1} f(x, y) \mu_1(dx) \right) \mu_2(dy). \end{aligned}$$

If $f: X \rightarrow \mathbb{C}$ then the above holds if one assumes in addition that

$$\int_{X_1 \times X_2} |f(x, y)| (\mu_1 \times \mu_2)(dx dy) < \infty.$$

2.2.2. *The layer-cake representation.* Let (X, μ) be a measure space and $f: X \rightarrow \mathbb{C}$ measurable. Define the function $\lambda_f: \mathbb{R}_+ \rightarrow [0, \infty]$,

$$\lambda_f(t) := \mu(\{x \in X : |f(x)| > t\}),$$

and its formal differential (the sign because λ_f is decreasing)

$$d\lambda_f(t) := -\mu(\{x \in X : |f(x)| = t\}).$$

These allow to express the properties of f in terms of layers of its graph or its level sets, namely, using that

$$|f(x)|^p = \int_{t=0}^{\infty} \mathbb{1}_{\{|f(x)|>t\}} d(t^p),$$

with $d(t^p) = pt^{p-1}dt$, one has the **layer-cake representation**

$$\|f\|_p^p = \int_{t=0}^{\infty} \lambda_f(t) d(t^p) = \int_{t=\infty}^0 t^p d\lambda_f(t), \quad (2.5)$$

where the second identity is a formal partial integration. Also,

$$\|f\|_{\infty} = \inf\{t \geq 0 : \lambda_f(t) = 0\}.$$

An immediate application of (2.5) is **Chebyshev's inequality**

$$\|f\|_p^p \geq t^p \lambda_f(t), \quad \forall t \geq 0. \quad (2.6)$$

2.3. Fourier transform. Given a measurable function $f: \mathbb{R}^n \rightarrow \mathbb{C}$, we formally define its **Fourier transform** \hat{f} by

$$\hat{f}(\xi) := (\mathcal{F}f)(\xi) := (2\pi)^{-n/2} \int_{\mathbb{R}^n} f(x) e^{-i\xi \cdot x} dx.$$

It can be shown that \mathcal{F} is a bijective (and obviously linear) map from $L^2(\mathbb{R}^n)$ into itself, with its inverse given by

$$f(x) = (\mathcal{F}^{-1}\hat{f})(x) := (2\pi)^{-n/2} \int_{\mathbb{R}^n} \hat{f}(\xi) e^{i\xi \cdot x} d\xi.$$

Moreover, **Plancherel's identity**

$$\|\mathcal{F}f\|_{L^2(\mathbb{R}^n)} = \|f\|_{L^2(\mathbb{R}^n)}, \quad f \in L^2(\mathbb{R}^n),$$

shows that \mathcal{F} is a **unitary** map on $L^2(\mathbb{R}^n)$, i.e. its adjoint satisfies $\mathcal{F}^* = \mathcal{F}^{-1}$.

We also have the important relations between differentiation and multiplication

$$\left(\frac{\partial f}{\partial x_j}\right)^{\wedge}(\xi) = i\xi_j \hat{f}(\xi), \quad (x_j f)^{\wedge}(\xi) = i\frac{\partial \hat{f}}{\partial \xi_j}(\xi), \quad j = 1, \dots, n. \quad (2.7)$$

2.4. Sobolev spaces. For any $s \geq 0$, we define the **Sobolev space** to be the space of square-integrable functions having square-integrable derivatives to order s , using the Fourier transform on \mathbb{R}^n and (2.7) as

$$H^s(\mathbb{R}^n) := \{f \in L^2(\mathbb{R}^n) : |\xi|^s \hat{f}(\xi) \in L^2(\mathbb{R}^n)\}. \quad (2.8)$$

The most common case is that $s = k$ is a non-negative integer, $H^k(\mathbb{R}^n)$, while otherwise the space is called a *fractional* Sobolev space. We note that $H^s(\mathbb{R}^n)$ is a Hilbert space with the inner product

$$\langle f, g \rangle_{H^s(\mathbb{R}^n)} := \int_{\mathbb{R}^n} \overline{\hat{f}(\xi)} \hat{g}(\xi) (1 + |\xi|^2)^s d\xi. \quad (2.9)$$

In particular, given a subset $\Omega \subseteq \mathbb{R}^n$, one may consider the subspace $C_c^\infty(\Omega) \subseteq H^s(\mathbb{R}^n)$ of smooth and compactly supported functions on Ω and take its closure in $H^s(\mathbb{R}^n)$ (with respect to the norm induced from the above inner product). We denote this space

$$H_0^s(\Omega) := \{f \in H^s(\mathbb{R}^n) : \exists (f_n) \subset C_c^\infty(\Omega), \|f_n - f\|_{H^s(\mathbb{R}^n)} \rightarrow 0\}, \quad (2.10)$$

and it has the interpretation as the space of functions which vanish ‘sufficiently fast’ at the boundary $\partial\Omega$ (and are identically zero on Ω^c). One has $H_0^s(\mathbb{R}^n) = H^s(\mathbb{R}^n)$.

It is important to know that it is possible to define Sobolev spaces locally, i.e. on domains $\Omega \subseteq \mathbb{R}^n$, without the use of the Fourier transform, however we will not discuss this properly here since it is most naturally done using the theory of distributions which goes beyond the course prerequisites. We only mention that, given $u \in L_{\text{loc}}^1(\Omega) \supseteq L_{\text{loc}}^{p \geq 1}(\Omega)$ it is always possible to define its gradient ∇u as a generalized function, and in the case that this turns out to be a locally integrable function, i.e. $\nabla u \in L_{\text{loc}}^1(\Omega; \mathbb{C}^n)$, we say that u is **weakly differentiable** (it has weak partial derivatives $\partial_j u \in L_{\text{loc}}^1(\Omega)$, $j = 1, \dots, n$). It may even turn out that $\nabla u \in L^q(\Omega; \mathbb{C}^n)$ for some $q \geq 1$, and we define the Sobolev spaces

$$H^1(\Omega) := \{u \in L^2(\Omega) : u \text{ is weakly differentiable and } \nabla u \in L^2(\Omega; \mathbb{C}^n)\}$$

and, by iteration of this procedure to higher orders of derivatives, for $k \in \mathbb{N}$

$$H^k(\Omega) := \{u \in L^2(\Omega) : u \text{ has weak partial derivatives all the way up to order } k, \text{ and} \\ \text{all of which are in } L^2(\Omega)\}.$$

The inner product in this space is given by

$$\langle f, g \rangle_{H^k(\Omega)} = \int_{\Omega} \left(\overline{f(x)}g(x) + \sum_{\alpha} \overline{\partial_{\alpha} f(x)} \partial_{\alpha} g(x) \right) dx,$$

where the sum runs over all partial derivatives (α a multi-index) up to order k .

In the case $\Omega = \mathbb{R}^n$ these spaces turn out to coincide with the above definitions (2.8) and (2.10). When $\Omega \subsetneq \mathbb{R}^n$ they contain but may (or may not) differ from $H_0^k(\Omega)$, depending on the geometry of Ω (we will return to this question in Section 4.2), and will be associated to Neumann respectively Dirichlet boundary conditions for the Laplace operator.

Exercise 2.6. *Show that the norm in $H^k(\mathbb{R}^n)$ is equivalent to that defined by replacing the weight factor $w(\xi) = (1 + |\xi|^2)^k$ in (2.9) by $w_1(\xi) = 1 + |\xi|^{2k}$ or $w_2(\xi) = 1 + \sum_{j=1}^n |\xi_j|^{2k}$.*

2.5. Forms and operators. An **operator** on a Hilbert space \mathcal{H} is a linear map $A: \mathcal{D}(A) \rightarrow \mathcal{H}$, with the subspace $\mathcal{D}(A) \subseteq \mathcal{H}$ the **domain** of A . Let $\|A\| := \sup_{u \in \mathcal{D}(A): \|u\|=1} \|Au\|$, then A is called **bounded** if $\|A\| < \infty$ and **unbounded** otherwise, and **closed** if its graph

$$\Gamma(A) := \{(u, v) \in \mathcal{D}(A) \times \mathcal{H} : v = Au\}$$

is a closed subspace of $\mathcal{H} \times \mathcal{H}$. We will always work with densely defined operators, i.e. with $\mathcal{D}(A)$ dense in \mathcal{H} , and shall denote by $\mathcal{L}(\mathcal{H})$ the space of such operators on \mathcal{H} . We have a subspace $\mathcal{B}(\mathcal{H}) \subseteq \mathcal{L}(\mathcal{H})$ of bounded operators A , for which one may assume $\mathcal{D}(A) = \mathcal{H}$.

An operator $A \in \mathcal{L}(\mathcal{H})$ is **hermitian** (or **symmetric**) if its corresponding sesquilinear form

$$\mathcal{D}(A) \times \mathcal{D}(A) \rightarrow \mathbb{C}, \quad (u, v) \mapsto \langle u, Av \rangle \quad (2.11)$$

satisfies $\langle u, Av \rangle = \langle Au, v \rangle$ for all $u, v \in \mathcal{D}(A)$ (compare Definition 2.1.(iii)). Hermitian operators are always **closable**, i.e. there is an **extension** $\hat{A}: \mathcal{D}(\hat{A}) \rightarrow \mathcal{H}$, with $\mathcal{D}(\hat{A}) \supseteq \mathcal{D}(A)$ and $\hat{A}|_{\mathcal{D}(A)} = A$, which is closed. Every closable operator A has a smallest closed extension, its **closure** \bar{A} , and every hermitian operator has a largest (on \mathcal{H}) closed extension, namely its **adjoint** A^* , which is in general defined with the domain

$$\mathcal{D}(A^*) := \left\{ u \in \mathcal{H} : \sup_{v \in \mathcal{D}(A): \|v\|=1} |\langle u, Av \rangle| < \infty \right\}$$

and (via the Riesz lemma) the formula $\langle u, Av \rangle = \langle A^*u, v \rangle$ for all $u \in \mathcal{D}(A^*)$, $v \in \mathcal{D}(A)$. The operator A is called **self-adjoint** if $A^* = A$, i.e. if $\mathcal{D}(A^*) = \mathcal{D}(A)$ and it is hermitian, and **essentially self-adjoint** if it is hermitian and has a unique self-adjoint extension $\bar{A} = A^*$. Any bounded hermitian operator is self-adjoint.

Example 2.10. The Laplace operator $L: u \mapsto -u''$ on the interval $[0, 1]$ is unbounded and not defined as an operator on the full Hilbert space $L^2([0, 1])$, but its restriction $L|_{C_c^\infty([0,1])}$ to the smooth functions with compact support (usually referred to as the **minimal domain**) is perfectly well-defined and hermitian. Its closure $\bar{L}|_{C_c^\infty([0,1])} = L|_{H_0^2([0,1])}$ is not self-adjoint, $L|_{H_0^2([0,1])}^* = L|_{H^2([0,1])}$, however it has several self-adjoint extensions, such as the **Dirichlet Laplacian** $-\Delta^D := L|_{\mathcal{D}(-\Delta^D)}$, with

$$\mathcal{D}(-\Delta^D) := \{u \in H_0^1([0, 1]) : u' \in H^1([0, 1])\} = H_0^1([0, 1]) \cap H^2([0, 1]),$$

and the **Neumann Laplacian** $-\Delta^N := L|_{\mathcal{D}(-\Delta^N)}$, with

$$\mathcal{D}(-\Delta^N) := \{u \in H^1([0, 1]) : u' \in H_0^1([0, 1])\} \subsetneq H^2([0, 1]).$$

In contrast, when considering L on the full real line, $L|_{C_c^\infty(\mathbb{R})}$ is essentially self-adjoint in $L^2(\mathbb{R})$, with $\bar{L}|_{C_c^\infty(\mathbb{R})} = L|_{H^2(\mathbb{R})}$. This follows from the properties of Sobolev spaces, namely $H_0^2(\mathbb{R}^2) = H^2(\mathbb{R}^2)$.

The form (2.11) of an operator A usually extends to a larger dense subspace $\mathcal{Q}(A) \subseteq \mathcal{H}$ called a **form domain** of A . We extend the notion of quadratic form to the unbounded case, just as in Definition 2.1 but with V replaced by a dense subspace $\mathcal{D}(q) \subseteq \mathcal{H}$, $q: \mathcal{D}(q) \rightarrow \mathbb{C}$. In particular, it is **hermitian** if $q: \mathcal{D}(q) \rightarrow \mathbb{R}$, **non-negative** if $q: \mathcal{D}(q) \rightarrow \mathbb{R}_+$, and **strictly positive** if $q(u) > 0$ for all $u \in \mathcal{D}(q) \setminus \{0\}$. We can also compare two hermitian quadratic forms q and q' if their domains intersect, and say that $q \geq q'$ iff $\mathcal{D}(q) \subseteq \mathcal{D}(q')$ and $q(u) \geq q'(u)$ for all $u \in \mathcal{D}(q)$. Thus the form q is **semi-bounded from below** if $q \geq c$ for some constant $c \in \mathbb{R}$, i.e. $q(u) \geq c\|u\|^2$ for all $u \in \mathcal{D}(q)$. Note that if $c < 0$ such a form can always be converted to a non-negative one by adding to it the constant $-c$. Furthermore, for semi-bounded forms we usually distinguish the domain by writing $q(u) = +\infty$ iff $u \notin \mathcal{D}(q)$.

A non-negative (or semi-bounded with the above trick) quadratic form is said to be **closed** iff $\mathcal{D}(q)$ is complete in the form norm $\|u\|_{q+1}^2 := q(u) + \|u\|^2$. The following then gives a very useful correspondence between forms and operators (cf. Exercise 2.8):

Theorem 2.11 (see e.g. [Tes14, Theorem 2.14]). *If the quadratic form $q: \mathcal{D}(q) \rightarrow \mathbb{R}$ is semi-bounded and closed, then it is the form $q|_{\mathcal{D}(A)} = q_A$, with $q_A(u) := \langle u, Au \rangle$, of a unique*

self-adjoint, semi-bounded operator A . Furthermore, A is given by

$$\mathcal{D}(A) = \left\{ u \in \mathcal{D}(q) : \exists u_q \in \mathcal{H} \text{ s.t. } \langle v, u \rangle_q = \langle v, u_q \rangle \forall v \in \mathcal{D}(q) \right\}, \quad Au = u_q.$$

The form domain of A is therefore $\mathcal{Q}(A) := \mathcal{D}(q)$, to which q_A extends as the closed form q . It also follows that for semi-bounded hermitian operators there is always a unique self-adjoint extension associated to the form (2.11), called the **Friedrichs extension**.

Theorem 2.12 (Friedrichs extension; see e.g. [RS75, Theorem X.23] or [Tes14, §2.3]). *For any semi-bounded from below hermitian operator A , the quadratic form $q_A(u) := \langle u, Au \rangle$ with $\mathcal{D}(q_A) = \mathcal{D}(A)$ is closable and its closure $\overline{q_A} = q_{\hat{A}_F}$ is the quadratic form of a unique semi-bounded self-adjoint operator \hat{A}_F . Furthermore, \hat{A}_F is the only self-adjoint extension \hat{A} of A s.t. $\mathcal{D}(\hat{A}) \subseteq \mathcal{D}(\overline{q_A}) =: \mathcal{Q}(\hat{A}_F)$ and the largest ($\hat{A}_F \geq \hat{A}$, i.e. $\mathcal{D}(\hat{A}_F) \subseteq \mathcal{D}(\hat{A})$) among all semi-bounded self-adjoint extensions of A .*

Note that we compare semi-bounded hermitian operators in terms of their quadratic forms: $A \geq B$ iff $\mathcal{D}(A) \subseteq \mathcal{D}(B)$ and $q_A \geq q_B$ on $\mathcal{D}(A)$.

Example 2.13. Associated to the Laplace operator L on $[0, 1]$ in Example 2.10 is the non-negative quadratic form $q_L(u) = \int_0^1 |u'|^2 dx$. The Dirichlet Laplacian $-\Delta^D$ is the Friedrichs extension of $L|_{C_c^\infty([0,1])}$ and thus also the operator associated to the closure of $q_L|_{C_c^\infty([0,1])}$, with the resulting form domain $\mathcal{Q}(-\Delta^D) = H_0^1([0, 1])$, while the Neumann Laplacian $-\Delta^N$ is the operator associated to the closure of $q_L|_{C^\infty([0,1])}$, with resulting form domain $\mathcal{Q}(-\Delta^N) = H^1([0, 1])$. We have $-\Delta^D \geq -\Delta^N$ since $C_c^\infty \subseteq C^\infty$.

Although necessary for some parts of the course, we will for simplicity try to avoid operator theory as much as possible and will typically be working with forms and form domains instead of operators and operator domains. So for example if $u \in H^1(\Omega)$ and we write

$$\langle u, (-\Delta)u \rangle_{L^2(\Omega)}$$

then since $-\Delta = \nabla^* \nabla$, here with $\mathcal{Q}(-\Delta) = \mathcal{D}(\nabla) = H^1(\Omega)$ understood, we actually mean

$$\langle \nabla u, \nabla u \rangle_{L^2(\Omega)} = \int_{\Omega} |\nabla u|^2 < \infty.$$

Exercise 2.7. *Verify the statements in Example 2.10 (as completely as you can with the preliminaries at hand; you may e.g. use that any $u \in H^1([0, 1])$ is a continuous function on $(0, 1)$; see e.g. [Tes14, §2.7]).*

Exercise 2.8. *Suppose $q: \mathcal{H} \rightarrow \mathbb{C}$ is a bounded quadratic form, i.e. $|q(u)| \leq C \|u\|^2$. Show that there is a unique bounded operator A s.t. $\langle u, v \rangle_q = \langle u, Av \rangle$, and moreover that the norm of A is given by*

$$\|A\| = \sup_{\|u\|=\|v\|=1} |\langle u, Av \rangle| \leq 2C.$$

(The factor 2 may be removed in the hermitian case.)

2.5.1. *The spectral theorem.* The **spectrum** $\sigma(A)$ of an operator $A \in \mathcal{L}(\mathcal{H})$ is the set of points $\lambda \in \mathbb{C}$ for which there does not exist a bounded inverse to the operator $A - \lambda = A - \lambda \mathbb{1}$. For $\lambda \notin \sigma(A)$ we call such $(A - \lambda)^{-1}$ the **resolvent** of A at λ . A point $\lambda \in \sigma(A)$ is an **eigenvalue** of A if there is a corresponding nontrivial **eigenspace** $\ker(A - \lambda) \neq 0$ of **eigenvectors** $u \in \ker(A - \lambda) \setminus \{0\}$. An operator A is self-adjoint if and only if it is hermitian and $\sigma(A) \subseteq \mathbb{R}$.

To fully describe a self-adjoint operator in terms of its spectrum, one needs to have also a notion of spectral measure. A **projection-valued measure** P is a function $\Omega \mapsto P_\Omega$ on the Borel⁽³⁾ sets $\Omega \subseteq \mathbb{R}$ such that each P_Ω is a projection on a Hilbert space \mathcal{H} , $P_\emptyset = 0$, $P_\mathbb{R} = \mathbb{1}$, $P_{\Omega_1} P_{\Omega_2} = P_{\Omega_1 \cap \Omega_2}$, and if $\Omega = \cup_{n=1}^N \Omega_n$, with Ω_n and Ω_m disjoint for $n \neq m$, then $P_\Omega = s\text{-}\lim_{N \rightarrow \infty} \sum_{n=1}^N P_{\Omega_n}$. Given any $u, v \in \mathcal{H}$, we then have a complex measure $\Omega \mapsto \langle u, P_\Omega v \rangle$ on the real line.

Theorem 2.14 (Spectral theorem; see e.g. [RS72, Theorem VIII.6] or [Tes14, §3.1]). *There is a one-to-one correspondence between projection-valued measures P^A and self-adjoint operators $A = \int_{-\infty}^{\infty} \lambda dP^A(\lambda)$, with*

$$\mathcal{D}(A) := \left\{ u \in \mathcal{H} : \int_{-\infty}^{\infty} |\lambda|^2 d(\langle u, P^A u \rangle)(\lambda) < \infty \right\}$$

and

$$\langle u, Av \rangle = \int_{-\infty}^{\infty} \lambda \langle u, dP^A(\lambda)v \rangle := \int_{-\infty}^{\infty} \lambda d(\langle u, P^A v \rangle)(\lambda).$$

Furthermore,

$$\mathcal{Q}(A) = \left\{ u \in \mathcal{H} : \int_{-\infty}^{\infty} |\lambda| d(\langle u, P^A u \rangle)(\lambda) < \infty \right\} = \mathcal{D}(\sqrt{|A|})$$

and if $f: \mathbb{R} \rightarrow \mathbb{R}$ is a Borel function then we can define the operator

$$f(A) = \int_{-\infty}^{\infty} \lambda dP^{f(A)}(\lambda) := \int_{-\infty}^{\infty} f(\lambda) dP^A(\lambda).$$

One may decompose the spectrum of a self-adjoint operator A into either

$$\sigma(A) = \sigma_{\text{disc}}(A) \sqcup \sigma_{\text{ess}}(A) \quad \text{or} \quad \sigma(A) = \overline{\sigma_{\text{pp}}(A)} \cup \sigma_{\text{ac}}(A) \cup \sigma_{\text{sc}}(A)$$

(the latter sets may overlap), where the **discrete spectrum**

$$\sigma_{\text{disc}}(A) := \{ \lambda \in \sigma(A) : \dim P_{(\lambda-\epsilon, \lambda+\epsilon)}^A \mathcal{H} < \infty \text{ for some } \epsilon > 0 \}$$

is the set of isolated eigenvalues of finite multiplicity and the rest is the **essential spectrum**

$$\sigma_{\text{ess}}(A) := \{ \lambda \in \sigma(A) : \dim P_{(\lambda-\epsilon, \lambda+\epsilon)}^A \mathcal{H} = \infty \text{ for every } \epsilon > 0 \}$$

(usually referred to as the continuous part of the spectrum), while the **pure point spectrum** σ_{pp} is the set of all eigenvalues of A , and σ_{ac} resp. σ_{sc} are the supports for the **absolutely** resp. **singular continuous** parts of the spectral measure of A .

⁽³⁾The σ -algebra of **Borel sets** on a topological space is the smallest σ -algebra containing all open sets. A real-valued function f is a **Borel function** if $f^{-1}((a, b))$ is a Borel set for any interval (a, b) .

Example 2.15. An operator A with eigenvalues $(\lambda_j)_{j=0}^\infty \subset \mathbb{R}$ and a corresponding orthonormal basis of eigenfunctions $(u_j)_{j=0}^\infty \subset \mathcal{H}$ can be written $A = \int_{-\infty}^\infty \lambda dP^A(\lambda)$ with projection-valued measure $P^A = \sum_{j=0}^\infty \delta_{\lambda_j} u_j \langle u_j, \cdot \rangle$. Note that if $\lambda_1 = \lambda_2 = \dots = \lambda_N$ is a repeated eigenvalue then $\sum_{j=1}^N \delta_{\lambda_j} u_j \langle u_j, \cdot \rangle = \delta_{\lambda_1} P_W$, where P_W is the orthogonal projection on the eigenspace $W = \text{Span}\{u_j\}_{j=1}^N$.

Example 2.16. A **multiplication operator** on $L^2(\mathbb{R})$ by $f: \mathbb{R} \rightarrow \mathbb{R}$, $(A_f u)(x) := f(x)u(x)$ has formally

$$A_f = \int_{-\infty}^\infty f(\lambda) \delta_\lambda \langle \delta_\lambda, \cdot \rangle d\lambda, \quad \text{i.e.} \quad \langle u, A_f v \rangle = \int_{-\infty}^\infty f(\lambda) \overline{u(\lambda)} v(\lambda) d\lambda,$$

and $\sigma(A_f) = \overline{f(\mathbb{R})}$. Sometimes we shall identify the operator A_f with f , or, in accordance with common conventions, denote it \hat{f} (*not* the Fourier transform here).

The lowest eigenvalues $\lambda_1(A) \leq \lambda_2(A) \leq \dots < \inf \sigma_{\text{ess}}(A)$ (also ordered according to their multiplicity) of a semi-bounded from below self-adjoint⁽⁴⁾ operator A can be obtained using the so-called **min-max principle**:

$$\lambda_k(A) = \inf_{W_k} \sup_{u \in W_k \setminus \{0\}} \frac{\langle u, Au \rangle}{\|u\|^2}, \quad (2.12)$$

where the $W_k \subseteq \mathcal{H}$ are linear subspaces of $\mathcal{D}(A)$ such that $\dim W_k = k$. If $A \geq B$ then $\lambda_k(A) \geq \lambda_k(B)$ for each k , and $\inf \sigma_{\text{ess}}(A) \geq \inf \sigma_{\text{ess}}(B)$. The domain $\mathcal{D}(A)$ can in the above be replaced by the form domain $\mathcal{Q}(A)$, or even a dense subspace w.r.t. the form norm, such as typically C_c^∞ or C^∞ .

Furthermore, if one continues to evaluate (2.12) for $k = 1, 2, \dots$ and eventually only repeated values $\lambda_n = \lambda_{n+1} = \lambda_{n+2} = \dots$ are obtained, then one has reached the bottom of the essential spectrum, $\lambda_n = \inf \sigma_{\text{ess}}(A)$.

Example 2.17. Computing (2.12) with $A = L$ from Examples 2.10 and 2.13, i.e. $\langle u, Lu \rangle = \int_0^1 |u'|^2$ on the form domain $H_0^1([0, 1])$ or $C_c^\infty([0, 1])$ gives the eigenvalues λ of the Dirichlet Laplacian,

$$-u''(x) = \lambda u(x), \quad u(0) = u(1) = 0,$$

i.e. $u_n(x) \propto \sin(\pi n x)$, $\lambda_n = \pi^2 n^2$, $n = 1, 2, 3, \dots$. On the other hand, taking the form domain $H^1([0, 1])$ or $C^\infty([0, 1])$ gives those of the Neumann Laplacian,

$$-u''(x) = \lambda u(x), \quad u'(0) = u'(1) = 0,$$

i.e. $u_n(x) \propto \cos(\pi n x)$, $\lambda_n = \pi^2 n^2$, $n = 0, 1, 2, \dots$

Exercise 2.9. Given $-\Delta_{\mathbb{R}^d}$ on $L^2(\mathbb{R}^d)$ with domain $H^2(\mathbb{R}^d)$, find its spectral decomposition using the Fourier transform and its powers $(-\Delta_{\mathbb{R}^d})^s$ for $s > 0$ using the spectral theorem.

⁽⁴⁾Or just hermitian, for which the spectrum analyzed is that of its Friedrichs extension.

2.5.2. *Stone's theorem.* Crucially for quantum mechanics, **Stone's theorem** tells us that self-adjoint operators are the generators of groups of unitary transformations.

Theorem 2.18 (Stone's theorem; see e.g. [RS72, Theorem VIII.7-8] or [Tes14, §5.1]). *Let $A \in \mathcal{L}(\mathcal{H})$ be a self-adjoint operator and define $U(t) = e^{itA}$ (using the spectral theorem). Then $U(t)$ is a **strongly continuous one-parameter unitary group**, i.e.*

- (i) $U(t)$ is unitary for all $t \in \mathbb{R}$,
- (ii) $U(t+s) = U(t)U(s)$ for all $s, t \in \mathbb{R}$, and
- (iii) if $\psi \in \mathcal{H}$ and $t \rightarrow t_0$ then $(U(t) - U(t_0))\psi \rightarrow 0$.

Furthermore,

- (iv) if $\lim_{t \rightarrow 0} (U(t) - \mathbf{1})\psi/t$ exists, then $\psi \in \mathcal{D}(A)$, and
- (v) for such ψ , $(U(t) - \mathbf{1})\psi/t \rightarrow iA\psi$ as $t \rightarrow 0$.

Conversely, if $U(t)$ is a strongly continuous one-parameter unitary group acting on \mathcal{H} , then there is a self-adjoint operator $A \in \mathcal{L}(\mathcal{H})$ s.t. $U(t) = e^{itA}$.

In fact, strong continuity may be replaced by just *weak* continuity, since weak convergence implies strong convergence in this case; cf. [Tes14, Theorem 5.3] and [RS72, Theorem VIII.9].

3. A VERY BRIEF MATHEMATICAL FORMULATION OF CLASSICAL AND QUANTUM MECHANICS

We do not assume familiarity with classical and quantum physics in this course, and therefore give a very brief account of the essentials here. However, a deeper understanding of these concepts is of course helpful in the broader perspective and we refer to [Thi03, Thi02] and [Thi07, Part IV] for introductory material suitable for mathematicians. In Section 3.2 we discuss the question of stability of matter in classical mechanics, and in Section 3.6.1 we define what is meant with stability in quantum mechanics. Anyone who is already familiar with many-body quantum mechanics may safely skip the chapter except possibly for these parts.

3.1. Some classical mechanics. Although it is important to know that there are several different equivalent formulations of classical mechanics, with their own advantages and disadvantages, we here choose to take the shortest mathematical path to quantum mechanics, via Poisson algebras and Hamiltonian mechanics.

3.1.1. *Phase space and Poisson brackets.*

Definition 3.1 (Poisson algebra). A **Poisson algebra** \mathcal{A} is a vector space over \mathbb{F} (\mathbb{R} or \mathbb{C}) equipped with an \mathbb{F} -bilinear and associative product

$$\mathcal{A} \times \mathcal{A} \rightarrow \mathcal{A}, \quad (f, g) \mapsto fg,$$

and an additional product (typically non-associative, called a **Poisson bracket**)

$$\mathcal{A} \times \mathcal{A} \rightarrow \mathcal{A}, \quad (f, g) \mapsto \{f, g\},$$

satisfying, for all $\alpha, \beta \in \mathbb{F}$, and $f, g, h \in \mathcal{A}$:

- (i) linearity: $\{f, \alpha g + \beta h\} = \alpha\{f, g\} + \beta\{f, h\}$,
- (ii) antisymmetry: $\{f, g\} = -\{g, f\}$,
- (iii) Jacobi identity: $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$,
- (iv) Leibniz rule: $\{f, gh\} = \{f, g\}h + g\{f, h\}$.

Remark 3.2. \mathcal{A} may also be equipped with a **unit** $1 \in \mathcal{A}$ s.t. $f = 1f = f1$. Note that (i)+(ii) implies bilinearity, (i)+(ii)+(iii) means that the product $\{\cdot, \cdot\}$ is a **Lie bracket** and $(\mathcal{A}, \{\cdot, \cdot\})$ a **Lie algebra**, and (iv) that it acts as a derivation of the associative product.

The archetypical example of a Poisson algebra is the algebra $\mathcal{A} = C^\infty(\mathcal{P}^n)$ of smooth functions on the **classical $2n$ -dimensional phase space**

$$\mathcal{P}^n := \mathbb{R}^{2n} \ni (\mathbf{x}, \mathbf{p}) = (x_1, \dots, x_n, p_1, \dots, p_n), \quad (3.1)$$

endowed with the Poisson bracket

$$\{f, g\} := \sum_{j=1}^n \left(\frac{\partial f}{\partial x_j} \frac{\partial g}{\partial p_j} - \frac{\partial g}{\partial x_j} \frac{\partial f}{\partial p_j} \right). \quad (3.2)$$

The first half of the phase space,

$$\mathcal{C}^n := \mathbb{R}^n \ni \mathbf{x} = (x_1, \dots, x_n),$$

is called the **classical configuration space** and is parameterized by the **coordinates** or **position variables** x_j , while the second half, parameterized by **momentum variables** p_j , is considered dual or **conjugate** to \mathcal{C}^n via the Poisson brackets. Namely, note that by (3.2),

the coordinates and momenta satisfy the following simple relations called the **canonical Poisson brackets**:

$$\{x_j, x_k\} = 0, \quad \{p_j, p_k\} = 0, \quad \{x_j, p_k\} = \delta_{jk}1, \quad \forall j, k, \quad (3.3)$$

where the constant function 1 on \mathcal{P}^n is the unit in \mathcal{A} . Hence the x_j 's and p_k 's Poisson-commute individually, while p_j is Poisson-conjugate to x_j and vice versa (though note that there is a certain choice of orientation in the bracket, so the coordinates x_j 's should come first).

In the case that we allow for complex-valued functions on phase space, we note that \mathcal{A} is also (non-trivially) endowed with the structure of a ***-algebra** in the sense that there is an operation $f \mapsto f^*$, here given by complex-conjugation $f^*(x, p) := \overline{f(x, p)}$, satisfying:

- (i) $(\alpha f + \beta g)^* = \bar{\alpha}f^* + \bar{\beta}g^*$ (conjugate linear)
- (ii) $(f^*)^* = f$ (involution),
- (iii) $(fg)^* = g^*f^*$ (antiautomorphism).

Remark 3.3.* The proper mathematical setting for classical mechanics in general is to model the Poisson algebra $\mathcal{A} = C^\infty(\mathcal{P}^n)$ on a geometric object called a **symplectic manifold** (\mathcal{P}^n, ω) , where ω is a symplectic form. Then the Poisson bracket is $\{f, g\} := \chi_f(g)$, where the vector field $\chi_f \in T(\mathcal{P}^n)$ is defined via the relation $\omega(\chi_f, \cdot) = -df$. Typically, \mathcal{P}^n is defined as the cotangent bundle of a configuration space manifold $\mathcal{C}^n = \mathcal{M}$, $\dim \mathcal{M} = n$, i.e. $\mathcal{P}^n := T^*(\mathcal{M})$, with its canonical symplectic structure $\omega := d\theta$, $\theta[X](p) := p(\pi X)$, given locally by $\theta = \sum_{j=1}^n p_j dx_j$ and (3.2). See e.g. [Thi07, Nak03].

Exercise 3.1. Check that (3.2) defines a Poisson bracket and makes $\mathcal{A} = C^\infty(\mathcal{P}^n)$ a Poisson algebra. Discuss whether (3.3) also defines this Poisson algebra completely.

3.1.2. *Hamiltonian mechanics.* Classical mechanics is about time evolution on the configuration space \mathcal{C}^n , i.e. one considers maps

$$\mathbb{R} \supseteq I \rightarrow \mathcal{C}^n, \quad t \mapsto \mathbf{x}(t) = (x_1(t), \dots, x_n(t)).$$

The evolution is typically of second order in time but can instead be formulated in a more advantageous first-order form on the phase space \mathcal{P}^n if one takes as the momenta $p_j := \dot{x}_j$ (or similar), with the dot denoting the derivative with respect to time t , $\dot{f} := df/dt$.

The desired evolution equation is then determined by a choice of a function H on the phase space called the **Hamiltonian**, i.e. an element $H \in \mathcal{A}$ which depends on the particular physical system under consideration. The value of this function $H(x, p)$ can usually be interpreted as the energy of the system at the corresponding point (x, p) in the phase space. The time evolution for general $f \in \mathcal{A}$ is then defined to be governed by the equation

$$\boxed{\dot{f} = \{f, H\}}, \quad (3.4)$$

reducing in particular, by (3.2), for the case of the coordinates and momenta to **Hamilton's equations of motion**:

$$\dot{x}_j = \frac{\partial H}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial H}{\partial x_j}. \quad (3.5)$$

Note conversely that these equations and the definition (3.2) imply (3.4),

$$\dot{f} = \frac{d}{dt}f(\mathbf{x}, \mathbf{p}) = \sum_{j=1}^n \left(\frac{\partial f}{\partial x_j} \frac{dx_j}{dt} + \frac{\partial f}{\partial p_j} \frac{dp_j}{dt} \right) = \sum_{j=1}^n \left(\frac{\partial f}{\partial x_j} \frac{\partial H}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial H}{\partial x_j} \right) = \{f, H\}.$$

Example 3.4 (Free particle). A particle that is free to move in three-dimensional space has the configuration space $\mathcal{C}^3 = \mathbb{R}^3$ of positions $\mathbf{x} = (x_1, x_2, x_3)$ and the phase space $\mathcal{P}^3 = \mathbb{R}^6 \ni (\mathbf{x}, \mathbf{p})$, where $\mathbf{p} = (p_1, p_2, p_3)$ is the canonical momentum of the particle. These variables satisfy the canonical Poisson brackets (3.3). We take the Hamiltonian to be the (**non-relativistic**; see also the below remark for an explanation) **free kinetic energy**

$$H(\mathbf{x}, \mathbf{p}) = T(\mathbf{p}), \quad T(\mathbf{p}) := \frac{\mathbf{p}^2}{2m}, \quad (3.6)$$

with $m > 0$ known as the **mass** of the particle which is considered as a fixed (non-dynamical) parameter. Indeed, Hamilton's equations of motion (3.5) are then

$$\dot{\mathbf{x}} = \mathbf{p}/m, \quad \dot{\mathbf{p}} = 0,$$

i.e. $\ddot{\mathbf{x}} = 0$, giving straight trajectories $\mathbf{x}(t) = \mathbf{a} + t\mathbf{b}$ in \mathcal{C}^3 . Also, we obtain the relationship $\mathbf{p} = m\mathbf{v}$ between the momentum and the velocity $\mathbf{v} := \dot{\mathbf{x}}$ of the particle, and therefore the well-known formula for its kinetic energy

$$T(\mathbf{p}) = \frac{1}{2}m\mathbf{v}^2.$$

*Remark** 3.5. The special theory of relativity tells us that $(mc^2)^2 = E^2 - \mathbf{p}^2c^2$, where mc^2 is the rest energy, or m the rest mass, of a free particle. Therefore, for small $\mathbf{p}/(mc)$,

$$E = \sqrt{m^2c^4 + c^2\mathbf{p}^2} = mc^2 \sqrt{1 + \frac{\mathbf{p}^2}{m^2c^2}} = mc^2 + \frac{\mathbf{p}^2}{2m} + O(\mathbf{p}^4), \quad (3.7)$$

which after subtracting the constant mc^2 yields the non-relativistic (first-order) approximation (3.6) to the kinetic energy. However, one may also study the full relativistic expression $T_{\text{rel},m}(\mathbf{p}) := mc^2 \sqrt{1 + \mathbf{p}^2/(mc)^2} - mc^2$ or the simpler massless case $T_{\text{rel},0}(\mathbf{p}) := c|\mathbf{p}|$.

Example 3.6 (Particle in an external potential). Mechanics would be rather boring if there were only free particles moving in straight lines, but what we may do is to add a **scalar potential** to the Hamiltonian (3.6),

$$H(\mathbf{x}, \mathbf{p}) = T(\mathbf{p}) + V(\mathbf{x}),$$

where $V: \mathbb{R}^3 \rightarrow \mathbb{R}$ is a function of the coordinates only. Hamilton's equations are then modified to

$$\dot{\mathbf{x}} = \mathbf{p}/m, \quad \dot{\mathbf{p}} = -\nabla V,$$

where $\mathbf{F} := -\nabla V$ is the **force** acting on the particle, with its sign chosen to act to *minimize* the potential energy. Hence, $m\ddot{\mathbf{x}} = \mathbf{F}$, which is **Newton's equation of motion**.

*Remark** 3.7. In fact, the potential may be understood to have a geometric origin and is again most naturally formulated in the framework of relativity. Namely, one couples the spacetime momentum $\mathbf{p} = (E/c, \mathbf{p})$ of the particle to the **gauge potential** $A(\mathbf{x}) =$

$(A_0(t, \mathbf{x}), \mathbf{A}(t, \mathbf{x}))$ of the electromagnetic field $F = dA$ using the replacement $\mathbf{p} \mapsto \mathbf{p} - q\mathbf{A}$, where q is the charge of the particle. Then $(mc)^2 = (\mathbf{p} - q\mathbf{A})^2 = (E/c - qA_0)^2 - (\mathbf{p} - q\mathbf{A})^2$ implies the electromagnetically coupled version of (3.7):

$$E = mc^2 + \frac{(\mathbf{p} - q\mathbf{A})^2}{2m} + V + O((\mathbf{p} - q\mathbf{A})^4),$$

with scalar potential $V = qcA_0$. See [Nak03] for more on the geometry of electrodynamics.

Example 3.8 (Harmonic oscillator). The standard example of an external potential, due to its simplicity and also its widespread appearance in real physical systems, is the **harmonic oscillator potential**,

$$V_{\text{osc}}(\mathbf{x}) := \frac{1}{2}m\omega^2|\mathbf{x}|^2,$$

where $\omega \geq 0$ is a parameter known as the angular frequency of the oscillator. The mass m appears here scaled out of ω in order to make the dynamics independent of m , namely, Newton's equations become simply $\ddot{\mathbf{x}} = -\omega^2\mathbf{x}$, with well-known $2\pi\omega$ -periodic solutions.

What one usually does in preparation for the quantum version of the harmonic oscillator is to introduce the *complex* phase-space variables

$$a_j := \sqrt{\frac{m\omega}{2}} \left(x_j + \frac{i}{m\omega} p_j \right), \quad a_j^* = \sqrt{\frac{m\omega}{2}} \left(x_j - \frac{i}{m\omega} p_j \right).$$

One may then observe that these satisfy the Poisson algebra

$$\{a_j, a_k\} = 0, \quad \{a_j^*, a_k^*\} = 0, \quad \{a_j, a_k^*\} = -i\delta_{jk}1, \quad (3.8)$$

and, if $\mathcal{N} := \sum_j a_j^* a_j = \sum_j |a_j|^2$,

$$\mathcal{N} = \mathcal{N}^* = H/\omega, \quad \{\mathcal{N}, a_j\} = ia_j, \quad \{\mathcal{N}, a_j^*\} = -ia_j^*. \quad (3.9)$$

Also, $x_j = (2m\omega)^{-1/2}(a_j^* + a_j)$ and $p_j = i(m\omega/2)^{1/2}(a_j^* - a_j)$.

Note that by construction of the dynamical equations (3.4) and the antisymmetry of the Poisson bracket, we have that the Hamiltonian is a conserved quantity under the motion,

$$\frac{d}{dt}H(\mathbf{x}, \mathbf{p}) = \dot{H} = \{H, H\} = 0. \quad (3.10)$$

In fact, any function f on \mathcal{P}^n is by (3.4) conserved in time iff it Poisson-commutes with H (the general important relationship between symmetries of the Hamiltonian and conserved quantities admits a more thorough formulation and is known as Noether's theorem).

*Remark** 3.9. There are subtleties even in classical mechanics when one considers systems with singular behavior which need to be treated using **constraints**. Typical examples are field theories such as electromagnetism, where passing from a Lagrangian to a Hamiltonian formulation involves redundant degrees of freedom and results in non-invertible transformations. However, Dirac has invented a procedure to treat such constrained Hamiltonian systems and to perform reductions in the Poisson algebra. See [Dir67], [Thi07, Chapter 24], and e.g. [dWHL11] for a recent example in membrane theory. Also fully general-relativistic systems — where there is no canonical time coordinate — may be considered, though in an even more general framework for mechanics, as outlined e.g. in [Rov04, Thi07].

Exercise 3.2. Verify the brackets (3.8) and (3.9).

3.2. The instability of classical matter. Let us briefly discuss why ordinary matter formulated in terms of the above-outlined rules for mechanics turns out to be unstable. We do not need to construct a very complicated model of matter in order to see the instability. In fact it arises already upon considering the simplest model of an atom consisting of a single electron moving in three-dimensional space around a fixed nucleus, which we for simplicity place at the origin of the electron's coordinate system $\mathcal{C}^3 = \mathbb{R}^3$. To justify this assumption, either consider the nucleus to be much heavier than the electron (which indeed it is by experiment) so that it experiences only very slow acceleration (according to Newton's equation) and thus can be safely considered fixed during a short time frame, or better consider the problem in **relative coordinates** as will be described in Section 3.5.

The electron and the nucleus have opposite electric charge and therefore experience an attractive electric force given by the **Coulomb potential**,

$$V_C(\mathbf{x}) := \frac{q_1 q_2}{|\mathbf{x}|}, \quad (3.11)$$

where q_1 and q_2 are the particles' respective charges, resulting in the Coulomb force

$$\mathbf{F}_C(\mathbf{x}) = -\nabla V_C(\mathbf{x}) = q_1 q_2 \frac{\mathbf{x}}{|\mathbf{x}|^3}.$$

In accordance with commonly used conventions and for future simplicity, we will normalize the electron charge to $q_1 = -1$ and call the charge of the nucleus $q_2 = Z > 0$. For a *neutral* one-electron atom the nucleus consists of a single proton with charge $+1$ and we thus have $Z = 1$ (this charge Z is known in chemistry as the **atomic number**, with $Z = 1$ representing the hydrogen atom), however we will for generality keep $Z > 0$ free as a mathematical parameter. We therefore take as our model for the dynamics of the electron in this **hydrogenic atom** the model considered in Example 3.6, with the external potential⁽⁵⁾

$$V_C(\mathbf{x}) = -\frac{Z}{|\mathbf{x}|}.$$

Hence the Hamiltonian defined on the electron's phase space $\mathcal{P}^3 = \mathbb{R}^3 \times \mathbb{R}^3 \ni (\mathbf{x}, \mathbf{p})$ is

$$H(\mathbf{x}, \mathbf{p}) = T(\mathbf{p}) + V_C(\mathbf{x}) = \frac{\mathbf{p}^2}{2m} - \frac{Z}{|\mathbf{x}|}. \quad (3.12)$$

We already observe an obvious problem here: that H is *unbounded from below*, namely fixing \mathbf{p} while taking $\mathbf{x} \rightarrow 0$ results in $H(\mathbf{x}, \mathbf{p}) \rightarrow -\infty$. However, one may object that this limit is quite artificial and perhaps cannot be realized in practice, in particular because the energy must be conserved throughout the dynamics as we already observed in (3.10). Let us therefore instead consider a possible trajectory: say for simplicity that the electron starts from rest at the point $(1, 0, 0) \in \mathbb{R}^3$, i.e. $\mathbf{x}(0) = (1, 0, 0)$ and $\mathbf{p}(0) = \mathbf{0}$. Then the non-trivial equation of motion to be solved is

$$m\ddot{x}_1 = -Zx_1/|x_1|^3, \quad x_1(0) = 1, \quad \dot{x}_1(0) = 0, \quad (3.13)$$

whose solution (see Exercise 3.3) can be seen to satisfy $x_1(t) \rightarrow 0$ in finite time. Therefore the electron described in the framework of classical mechanics *admits dynamics whereby it collapses into the nucleus*.

⁽⁵⁾Though $V_C \notin \mathcal{A}$, we may consider it as a limit of smooth functions (see remark) or extend our \mathcal{A} a bit.

*Remark** 3.10. With a little more physics background, one may still object to this conclusion of instability in two ways. The first is that the nucleus is actually a composite particle which has some spatial extent and therefore it is not clear that a collapse happens — maybe the electron would just bounce around in a continuous charge distribution. However, it is known that the size of a nucleus is about 10^{-15} m while the typical size of a hydrogen atom is about 10^{-10} m (the Bohr radius), so from the perspective of the typical electron orbit the nucleus certainly looks pointlike, and one rather needs to explain why the electron insists on staying so far away from the nucleus. This leads to the second objection, namely that in analogy to the picture of a planetary system (which is completely justified from the model (3.12) since the Newtonian gravitational potential looks exactly the same), the electron could just move in a circular or elliptical orbit with its centripetal acceleration exactly matching the Coulomb force. In order to object to this picture of apparent stability one needs to know a little more about electromagnetic interactions, namely that an accelerating charge necessarily emits electromagnetic radiation to its surroundings (in order to properly incorporate this — still purely classical — effect, called *bremstrahlung*, one needs to modify both the above simple Hamiltonian and the phase space severely, and the resulting Hamiltonian describing the electron is then *not* conserved in time). The consequence of this radiative effect is that the electron loses energy and therefore transcends into lower and lower orbits, in effect spiraling in towards the nucleus and leading to the collapse of classical matter.

Exercise 3.3. Find an implicit solution of (3.13) for $x_1(t) > 0$ and determine the time T for which $x_1(T) = 0$. (*Hint: start by multiplying the equation by \dot{x}_1 .*)

3.3. Some quantum mechanics. The above-discussed problem of instability, together with other unexpected discoveries in the beginning of the 20th century, led to the realization that Hamiltonian mechanics on phase space (as well as the other equivalent formulations of classical mechanics) is not sufficient to describe the physical world. This was in the 1920's subsequently remedied by the invention of a *quantum* representation for mechanics. Nowadays this is quite well understood as a kind of mathematical recipe, referred to as **canonical quantization**, although depending on which systems are considered there are still many subtleties to be dealt with, both on a formal level and also when it comes to the physical interpretation.

3.3.1. Axioms of canonical quantization. In mathematical terms, the procedure of ‘canonical quantization’ amounts to selecting a (sufficiently interesting) Lie-subalgebra $\mathcal{O} \subseteq \mathcal{A}$ and a representation of this \mathcal{O} as an algebra of linear operators on a Hilbert space \mathcal{H} , $\mathcal{O} \rightarrow \hat{\mathcal{O}} \subseteq \mathcal{L}(\mathcal{H})$. This translates to the following set of **axioms of quantum mechanics**:

- A1. (States) There exists a complex⁽⁶⁾ separable⁽⁷⁾ Hilbert space \mathcal{H} , which we call the **quantum configuration space**. The non-zero elements $\psi \in \mathcal{H} \setminus \{0\}$ will describe the **states**⁽⁸⁾ of the quantum system, and furthermore two vectors ψ and ϕ in \mathcal{H} describe the same state if and only if $\phi = c\psi$, $c \in \mathbb{C} \setminus \{0\}$. In other words the set of quantum states constitutes a ray representation of \mathcal{H} .

⁽⁶⁾One may also consider purely real Hilbert spaces; see e.g. [Lun08] and references for a discussion.

⁽⁷⁾This assumption could, and should, sometimes be relaxed; see e.g. [Thi07, AS11].

⁽⁸⁾These may also be called **pure states** in contrast to **mixed states** (density matrices; Remark).

- A2. (Observables) One has selected a set of **observables** $a \in \mathcal{O}$ which form a closed Lie-subalgebra of \mathcal{A} , and which are real, $a^* = a$. To each such observable $a \in \mathcal{O}$ there is associated a densely defined self-adjoint operator \hat{a} acting on \mathcal{H} , i.e. $\hat{a}^* = \hat{a} \in \mathcal{L}(\mathcal{H})$. The spectrum of \hat{a} are the possible results of a measurement of the observable a .
- A3. (Commutators) The Poisson bracket in classical mechanics is replaced by the **commutator**

$$[\hat{a}, \hat{b}] := \hat{a}\hat{b} - \hat{b}\hat{a}$$

of operators, according to:

$$\{a, b\} \mapsto \frac{1}{i\hbar} [\hat{a}, \hat{b}]. \quad (3.14)$$

Here we have multiplied the commutator with $-i$ (and the sign is just a convention) in order to make the expression self-adjoint (by the closedness of \mathcal{O} , the bracket of two observables is also an observable and hence should be represented by a self-adjoint operator, but the commutator of two self-adjoint operators is *anti*-self-adjoint⁽⁹⁾), and we furthermore introduced a new parameter $\hbar > 0$ known as **Planck's constant**.

- A4. (Expectations) Given a state $\psi \in \mathcal{H}$, the **expectation value** of an observable $a \in \mathcal{O}$ in this state is given by

$$\langle \hat{a} \rangle_\psi := \frac{\langle \psi, \hat{a} \psi \rangle}{\langle \psi, \psi \rangle}.$$

The interpretation is that if one prepares a large ensemble of identical systems, each of which is prepared to be in the state ψ , and then makes a measurement of the observable a then the result of the measurement will in general be random but the expectation value of the results will be given by the quantity $\langle \hat{a} \rangle_\psi \in \mathbb{R}$. If a has physical meaning but $\psi \notin \mathcal{Q}(\hat{a})$ then ψ may be interpreted as an unphysical state.

- A5. (Time evolution) The choice of dynamics depends on the choice of a Hamiltonian $H \in \mathcal{O}$, which is represented as a self-adjoint **Hamiltonian operator** \hat{H} on \mathcal{H} . Operators corresponding to other observables may then evolve with time according to **Heisenberg's equation of motion** (compare (3.4)),

$$\frac{d}{dt} \hat{a}(t) = \frac{1}{i\hbar} [\hat{a}(t), \hat{H}], \quad (3.15)$$

and their corresponding expectation value at time t is

$$\langle \hat{a}(t) \rangle_\psi = \frac{\langle \psi, \hat{a}(t) \psi \rangle}{\langle \psi, \psi \rangle}.$$

Remark 3.11. The reasons for insisting that observables be represented by *self-adjoint* operators are threefold:

1. An observable $a \in \mathcal{O}$ should represent a real measurable physical quantity, and its expectation value satisfies $\langle \hat{a} \rangle_\psi \in \mathbb{R}$ for all states $\psi \in \mathcal{Q}(\hat{a})$ iff \hat{a} is hermitian.

⁽⁹⁾On the basis of this one may argue that the more natural thing to do is to replace everything by *anti*-self-adjoint operators.

2. Self-adjoint operators have a **spectral representation** given by the spectral theorem, Theorem 2.14, and the points of the spectrum $\sigma(\hat{a}) \subseteq \mathbb{R}$ represent the possible values of a measurement of the observable $a \in \mathcal{O}$. Also, if the system is in a state $\psi \in \mathcal{H}$, then the **probability** of measuring values of a in the interval $[\lambda, \lambda'] \subseteq \mathbb{R}$ is given by the expectation value (of the observable⁽¹⁰⁾ “ $a \in [\lambda, \lambda']$ ”)

$$\langle P_{[\lambda, \lambda']}^{\hat{a}} \rangle_{\psi} = \frac{\|P_{[\lambda, \lambda']}^{\hat{a}} \psi\|^2}{\|\psi\|^2}, \quad (3.16)$$

where $\Omega \mapsto P_{\Omega}^{\hat{a}}$ is the corresponding spectral projection (see e.g. Example 2.15).

3. By Stone’s theorem, Theorem 2.18, self-adjoint operators are the generators of one-parameter *unitary* groups, $t \mapsto U_{\hat{a}}(t) := e^{i\hat{a}t}$, which is in particular important for the time evolution by the Hamiltonian \hat{H} to *conserve* probabilities, $\|U_{\hat{H}}(t)\psi\| = \|\psi\|$. A *non-self-adjoint* Hamiltonian operator would describe *non-unitary* time evolution, which would however be appropriate when there is energy or **information loss** from the system to an external environment.

We also note that:

4. A **measurement** necessarily exchanges information between the system being measured and the observer, and therefore results in non-unitary evolution. In effect, after measurement the state has become projected into the subspace corresponding to the information obtained, $\psi \mapsto P_{[\lambda, \lambda']}^{\hat{a}} \psi$, by means of the spectral projection in (3.16). For example, if \hat{a} has an isolated simple eigenvalue $\lambda_j \in \sigma(\hat{a})$ with corresponding normalized eigenstate u_j , then the probability (3.16) of measuring precisely this value in the normalized state ψ is $\langle P_{[\lambda_j - \varepsilon, \lambda_j + \varepsilon]}^{\hat{a}} \rangle_{\psi} = |\langle u_j, \psi \rangle|^2$, and the state of the system $\psi \mapsto u_j$ after such a measurement. Repeated measurement of a will then produce the same value λ_j with certainty (unless the observable has evolved with time). The quantity $\langle u_j, \psi \rangle \in \mathbb{C}$ is called a **probability amplitude**, and the probabilistic interpretation is known as **Born’s rule**.

Remark 3.12. Instead of evolving the operators in time according to the solution of (3.15),

$$\hat{a}(t) = e^{it\hat{H}/\hbar} \hat{a}(0) e^{-it\hat{H}/\hbar} \in \mathcal{L}(\mathcal{H}),$$

one may evolve the states, $\psi(t) := e^{-it\hat{H}/\hbar} \psi(0) \in \mathcal{H}$, so that by unitarity

$$\langle \hat{a}(t) \rangle_{\psi(0)} = \langle \hat{a}(0) \rangle_{\psi(t)}.$$

These states then satisfy the **Schrödinger equation**

$$\boxed{i\hbar \frac{d}{dt} \psi(t) = \hat{H} \psi(t).}$$

⁽¹⁰⁾Note that if we can measure a then we may also determine if $a \in [\lambda, \lambda']$ for any interval $[\lambda, \lambda'] \subseteq \mathbb{R}$, and similarly if we have a self-adjoint operator \hat{a} then we also have access to its projection-valued measure $P_{[\lambda, \lambda']}^{\hat{a}}$. The commutativity of $P_{\Omega}^{\hat{a}}$ and $P_{\Omega'}^{\hat{b}}$ expresses what may be known simultaneously about a and b .

3.3.2. The Schrödinger representation. Let us now implement the above quantization rules on the archetypical Poisson algebra \mathcal{A} , namely the phase space (3.1)-(3.2), with the canonical Poisson brackets (3.3). We take the canonical coordinate and momentum functions x_j and p_k as our fundamental observables, with for example

$$\mathcal{O} = \text{Span}_{\mathbb{R}}\{1, x_1, \dots, x_n, p_1, \dots, p_n\}, \quad (3.17)$$

(note that we added 1 to make this a closed Lie-subalgebra of \mathcal{A} , also known as the Lie algebra of the **Heisenberg group**). However we will typically want to work with something slightly larger than (3.17) since by A5 we also need a Hamiltonian observable $H \in \mathcal{O}$ which is some function of \mathbf{x} and \mathbf{p} . These observables should according to A1-A2 be promoted to operators $\hat{1}, \hat{x}_j, \hat{p}_k \in \mathcal{L}(\mathcal{H})$ on some Hilbert space \mathcal{H} , which we leave undetermined for a brief moment.

The canonical Poisson brackets (3.3) should then according to A3 be represented by the **canonical commutation relations (CCR)**:

$$[\hat{x}_j, \hat{x}_k] = 0, \quad [\hat{p}_j, \hat{p}_k] = 0, \quad [\hat{x}_j, \hat{p}_k] = i\hbar \delta_{jk} \hat{1}. \quad (3.18)$$

We also note that since $\{1, a\} = 0$ for all $a \in \mathcal{A}$, we should have $[\hat{1}, \hat{a}] = 0$, at least for all $a \in \mathcal{O}$, so that upon considering irreducible⁽¹¹⁾ representations of this algebra we may write $\hat{1} = c\mathbb{1}$, where $c \in \mathbb{C}$, or actually $\bar{c} = c \in \mathbb{R}$ since $\hat{1}^* = \hat{1}$. However, as $\hat{1}$ appears only in combination with \hbar in the r.h.s. of (3.18), and since we have not yet fixed the value of \hbar , we may absorb this freedom into \hbar and take $c = 1$, i.e. $\hat{1} = \mathbb{1}$, the unit in $\mathcal{L}(\mathcal{H})$.

It is now time to find a Hilbert space on which to represent the operator observables. However, taking the simplest non-trivial choice that comes to mind, i.e. $\mathcal{H} = \mathbb{C}^N$ for some finite dimension $N \geq 1$ and with the operators acting as hermitian $N \times N$ -matrices, is seen not to work, simply by taking the trace on both sides of for example the operator equation corresponding to the first non-trivial commutator in (3.18),

$$\hat{x}_1 \hat{p}_1 - \hat{p}_1 \hat{x}_1 = i\hbar \mathbb{1}. \quad (3.19)$$

The trace is zero on the l.h.s. but $i\hbar N$ on the r.h.s., and hence yields a contradiction unless $\hbar = 0$. As a result, we cannot represent these relations non-trivially unless the space \mathcal{H} is *infinite*-dimensional, which leads us to the next-most natural choice $\mathcal{H} = L^2(\mathbb{C}^n) = L^2(\mathbb{R}^n)$, where we may for example take the standard **Schrödinger representation**: for $\psi \in \mathcal{H}$,

$$(\hat{x}_j \psi)(\mathbf{x}) := x_j \psi(\mathbf{x}), \quad (3.20)$$

i.e. simply multiplication by the coordinate, and

$$(\hat{p}_j \psi)(\mathbf{x}) := -i\hbar \frac{\partial \psi}{\partial x_j}(\mathbf{x}). \quad (3.21)$$

The sign convention on \hat{p}_j here matches that of (3.14).

Note that both of these are unbounded operators and therefore care has to be taken that they are self-adjoint. They are obviously hermitian when considered as forms on $C_c^\infty(\mathbb{R}^n)$,

$$\langle \varphi, \hat{x}_j \psi \rangle = \langle \hat{x}_j \varphi, \psi \rangle, \quad \langle \varphi, \hat{p}_k \psi \rangle = \langle \hat{p}_k \varphi, \psi \rangle, \quad \forall \varphi, \psi \in C_c^\infty(\mathbb{R}^n), \quad (3.22)$$

⁽¹¹⁾That is, if seen as matrices, not block-diagonalizable but restricted to just one full block which cannot be reduced further (no invariant strict subspace). Irreducibility comes in by axiom A1 and the desire to be able to distinguish all states. — If they are not distinguishable by any means then they should be identified!

but one needs to specify corresponding domains so that $\mathcal{D}(\hat{x}_j^*) = \mathcal{D}(\hat{x}_j)$ and $\mathcal{D}(\hat{p}_k^*) = \mathcal{D}(\hat{p}_k)$. In the case \hat{x}_j , the natural (maximal) domain is

$$\mathcal{D}(\hat{x}_j) := \left\{ \psi \in L^2(\mathbb{R}^n) : \int_{\mathbb{R}^n} |x_j|^2 |\psi(x)|^2 dx < \infty \right\},$$

while the common joint domain for all \hat{x}_j is

$$\mathcal{D}(\hat{x}) := \{ \psi \in L^2(\mathbb{R}^n) : \hat{x}\psi = (\hat{x}_1\psi, \dots, \hat{x}_n\psi) \in L^2(\mathbb{R}^n; \mathbb{C}^n) \},$$

and for \hat{p}_k ,

$$\mathcal{D}(\hat{p}_k) := \left\{ \psi \in L^2(\mathbb{R}^n) : \int_{\mathbb{R}^n} |\xi_k|^2 |\hat{\psi}(\xi)|^2 d\xi < \infty \right\}, \quad \mathcal{D}(\hat{p}) := H^1(\mathbb{R}^n). \quad (3.23)$$

This also corresponds to taking the closure of the minimal operators, i.e. with \hat{x}_j and \hat{p}_k initially defined on the minimal domain $C_c^\infty(\mathbb{R}^n)$.

Writing $p = \hbar\xi$ (we will later set $\hbar = 1$), we have in terms of the Fourier transform⁽¹²⁾ (2.7)

$$(\hat{p}_j\psi)^\wedge(p) = p_j\hat{\psi}(p), \quad (\hat{x}_k\psi)^\wedge(p) = i\hbar \frac{\partial \hat{\psi}}{\partial p_k}(p),$$

so that an alternative but equivalent representation (called the **momentum representation**) is given by $\mathcal{FH} = \mathcal{FL}^2(\mathbb{C}^n) = L^2(\mathbb{R}^n) \ni \hat{\psi}$ with operators $\check{I} = \mathbb{1}$, $\check{x}_k, \check{p}_j \in \mathcal{L}(\mathcal{FH})$ defined by

$$(\check{p}_j\hat{\psi})(p) := p_j\hat{\psi}(p), \quad (\check{x}_k\hat{\psi})(p) := i\hbar \frac{\partial \hat{\psi}}{\partial p_k}(p), \quad (3.24)$$

i.e. $\check{x}_k = \mathcal{F}\hat{x}_k\mathcal{F}^{-1}$ and $\check{p}_j = \mathcal{F}\hat{p}_j\mathcal{F}^{-1}$.

Remark 3.13 (Stone–von Neumann uniqueness theorem). In fact, one may consider the abstract unitary group generated by, say \hat{x}_1, \hat{p}_1 , with the commutation relations (3.19), via

$$U(s) := e^{is\hat{x}_1}, \quad V(t) := e^{it\hat{p}_1/\hbar}, \quad (3.25)$$

which satisfy the **Weyl algebra**

$$U(s)U(s') = U(s+s'), \quad V(t)V(t') = V(t+t'), \quad V(t)U(s) = e^{ist}U(s)V(t). \quad (3.26)$$

It turns out that, with the only assumptions that the representation of this group is unitary, irreducible and **weakly continuous**, i.e.

$$\lim_{t \rightarrow 0} \langle u, U(t)v \rangle = \langle u, v \rangle \quad \forall u, v \in \mathcal{H}, \quad (3.27)$$

and similarly for $V(t)$, it *must* be equivalent to the Schrödinger representation: that is, up to conjugation with a unitary (such as \mathcal{F}), we have $\mathcal{H} = L^2(\mathbb{R})$ with

$$(U(s)\psi)(x) = e^{isx}\psi(x), \quad (V(t)\psi)(x) = \psi(x+t). \quad (3.28)$$

This is known as the **Stone–von Neumann uniqueness theorem**. However, upon relaxing the assumption (3.27) on weak continuity other representations may be found, on *non-separable* Hilbert spaces; see Section 2.5.2 and [Thi07, p. 213], [AS11].

⁽¹²⁾The conventions here are unfortunate but standard; hats on states denote their Fourier transform, and otherwise it denotes operator representations of phase-space functions.

Since the \hat{x}_j are commuting operators we may diagonalize them simultaneously, with well-defined projections on the joint spectrum of the operators $\hat{x} = (\hat{x}_1, \dots, \hat{x}_n)$,

$$P_{I_1 \times I_2 \times \dots \times I_n}^{\hat{x}} = P_{I_1}^{\hat{x}_1} P_{I_2}^{\hat{x}_2} \dots P_{I_n}^{\hat{x}_n}, \quad I_j \subseteq \mathbb{R} \text{ intervals,}$$

which may be generalized to $P_{\Omega}^{\hat{x}}$ for any (Borel) $\Omega \subseteq \mathbb{R}^n$. This is again the same as taking the Schrödinger representation with $P_{\Omega}^{\hat{x}} = \mathbf{1}_{\Omega}$. For normalized $\psi \in L^2(\mathbb{R}^n)$, $\|\psi\|_{L^2} = 1$, we have by Remark 3.11.2 also a natural interpretation for

$$\int_{\Omega} |\psi|^2 = \langle \mathbf{1}_{\Omega} \rangle_{\psi} = \left\langle P_{\Omega}^{\hat{x}} \right\rangle_{\psi},$$

which is thus the probability of measuring the event $\mathbf{x} \in \Omega$ given the state $\psi \in \mathcal{H}$. Furthermore,

$$|\psi(\mathbf{x})|^2 = \langle \psi, \delta_{\mathbf{x}} \psi \rangle = \lim_{\varepsilon \rightarrow 0} |B_{\varepsilon}(\mathbf{x})|^{-1} \left\langle P_{B_{\varepsilon}(\mathbf{x})}^{\hat{x}} \right\rangle_{\psi}$$

(valid for a.e. $\mathbf{x} \in \mathbb{R}^n$ by the Lebesgue differentiation theorem) may be interpreted as the **probability density of measuring the coordinates** $\mathbf{x} \in \mathbb{R}^n$.

In the case of diagonalizing \hat{p} instead, i.e. switching to the momentum representation where $\mathcal{F} P_{\Omega}^{\hat{p}} \mathcal{F}^{-1} = P_{\Omega}^{\hat{p}} = \mathbf{1}_{\Omega}$, one has

$$|\hat{\psi}(\mathbf{p})|^2 = \left\langle \hat{\psi}, \delta_{\mathbf{p}} \hat{\psi} \right\rangle = \lim_{\varepsilon \rightarrow 0} |B_{\varepsilon}(\mathbf{p})|^{-1} \left\langle P_{B_{\varepsilon}(\mathbf{p})}^{\hat{p}} \right\rangle_{\hat{\psi}} = \lim_{\varepsilon \rightarrow 0} |B_{\varepsilon}(\mathbf{p})|^{-1} \left\langle P_{B_{\varepsilon}(\mathbf{p})}^{\hat{p}} \right\rangle_{\psi},$$

the **probability density of measuring the momenta** $\mathbf{p} \in \mathbb{R}^n$.

Remark 3.14. The reason why we cannot just take the full Poisson algebra $\mathcal{O} = \mathcal{A}$ and quantize that is that there will be problems when it comes to the choice of ordering of operators. Namely by (3.19), $\hat{x}_1 \hat{p}_1$ is not the same as $\hat{p}_1 \hat{x}_1$, so it matters if we by $x_1 p_1 = p_1 x_1 \in \mathcal{A}$ mean $\hat{x}_1 \hat{p}_1$, or $\hat{p}_1 \hat{x}_1$, or perhaps $\frac{1}{2}(\hat{x}_1 \hat{p}_1 + \hat{p}_1 \hat{x}_1)$. This is known as the **factor ordering ambiguity** in quantum mechanics and causes many headaches when trying to quantize classical mechanical systems. As a result there are often different routes to quantization with obstacles to be overcome and choices to be made of both ordering rules and representations, so that, in practice, the procedure of ‘canonical quantization’ may not seem so canonical after all. For a very general treatment of the quantization procedure, see e.g. [Thi07, Rov04].

Exercise 3.4. Verify (3.22) and the CCR (3.18) for both the choice (3.20)-(3.21) and the alternative (3.24), and note the agreement of all sign conventions.

Exercise 3.5. Verify that the Schrödinger representation (3.20)-(3.21) exponentiates to (3.28) and satisfies the Weyl algebra (3.26). Conjugate with \mathcal{F} and compare with (3.24). Derive the abstract Weyl algebra starting from the definitions (3.25) and the CCR (3.18).

3.4. The one-body problem. Let us now consider the case of the **one-body problem**, i.e. a single particle on a d -dimensional classical configuration space $\mathcal{C}^d = \mathbb{R}^d$ and phase space $\mathcal{P}^d = \mathbb{R}^{2d}$, on which we may take the Hamiltonian $H(\mathbf{x}, \mathbf{p}) = T(\mathbf{p}) + V(\mathbf{x})$ from Example 3.6 (in that case we had $d = 3$, but let us be more general here and take $d \in \mathbb{N}$). Since it generates our dynamics, we should promote it to an observable, i.e. add it to (3.17) and then construct its quantum representation $\hat{H} \in \mathcal{L}(\mathcal{H})$. However, before we do so, let

us make sure that we are done with our choice of observables \mathcal{O} . Namely, \mathcal{O} needs to be closed under Poisson brackets, and indeed

$$\{x_j, T(\mathbf{p})\} = \frac{p_j}{m} \in \mathcal{O}, \quad \{x_j, V(\mathbf{x})\} = 0, \quad \{p_j, T(\mathbf{p})\} = 0,$$

but we find that we might also need to add

$$\{p_j, V(\mathbf{x})\} = -\frac{\partial V(\mathbf{x})}{\partial x_j} = F_j(\mathbf{x}),$$

i.e. the components of the corresponding force \mathbf{F} , as well as

$$\{p_j, F_k(\mathbf{x})\} = -\frac{\partial F_k}{\partial x_j}(\mathbf{x}),$$

in case this expression is non-zero, and so on. Hence all of these functions on \mathcal{P}^d need to be represented as operators as well. Moreover, there may be other relevant observables such as

$$L_{jk} := x_j p_k - x_k p_j, \quad 1 \leq j < k \leq d, \quad (3.29)$$

for which $\{L_{jk}, T(\mathbf{p})\} = 0$ and $\{L_{jk}, V(\mathbf{x})\} = 0$ if $V(\mathbf{x}) = f(|\mathbf{x}|)$ (i.e. radial potentials), and which describe **angular momentum**. On the other hand, it is not always the case that any of the canonical variables x_j and p_k ought to be considered observables, and one may in such an extreme circumstance therefore just take the trivial choice $\mathcal{O} = \text{Span}\{1, H\}$ or $\mathcal{O} = \mathbb{R}H$ (but with e.g. some non-trivial representation based on the concrete expression for H) and hence only have to worry about quantizing the Hamiltonian H in that case.

Example 3.15 (Free particle). The simplest example is again the free particle with $V = 0$, for which we have $H = T(\mathbf{p}) = \mathbf{p}^2/(2m)$. In the usual Schrödinger representation (3.20)-(3.23) the natural thing to do is to take

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} = \frac{\hbar^2}{2m}(-\Delta_{\mathbb{R}^d}),$$

with domain $\mathcal{D}(\hat{H}) = \mathcal{D}(\hat{\mathbf{p}}^2) = H^2(\mathbb{R}^d)$. This is then a self-adjoint operator, and if instead considered on the minimal domain $C_c^\infty(\mathbb{R}^d)$ it is essentially self-adjoint with the above extension as its closure. Hence there is no other choice for the quantum dynamics in this case (there could however be other options if one changes \mathcal{C}^d a bit by for example removing or identifying points, as will be seen in Section 3.7). Moreover, taking the Fourier transform and thus the momentum representation as a pure multiplication operator (3.24) we may even determine its spectrum explicitly (cf. Exercise 2.9): $\sigma(\hat{H}) = \sigma(\hat{\mathbf{p}}^2/(2m)) = [0, \infty)$.

Even if the potential V is non-zero, since $T(\mathbf{p})$ and $V(\mathbf{x})$ depend only on \mathbf{p} and \mathbf{x} separately there is, luckily, no factor ordering problem in $H = T + V$. But we do need to ensure self-adjointness of \hat{H} , which could actually be quite difficult depending on V . The typical procedure would again be to use our earlier Schrödinger representation for $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}} = -i\hbar\nabla$ and thus write for the Hamiltonian operator

$$\hat{H} := T(\hat{\mathbf{p}}) + V(\hat{\mathbf{x}}) = T(-i\hbar\nabla) + V(\mathbf{x}) = \frac{\hbar^2}{2m}(-\Delta) + V(\mathbf{x}), \quad (3.30)$$

at least on the minimal domain $C_c^\infty(\mathbb{R}^d)$. This is a hermitian expression on this domain as long as the potential is real-valued, $V: \mathbb{R}^d \rightarrow \mathbb{R}$, and not too singular (as will be illustrated in Example 3.20), and one may consider it as the sum of two quadratic forms. In the case

that $V \geq -C$ with a constant $C \geq 0$ the resulting form is bounded from below, $\hat{H} \geq -C$, and therefore by Friedrichs extension, Theorem 2.12, there is a *unique* semi-bounded self-adjoint operator corresponding to the closure of this form expression. An operator on the form (3.30) for some potential V is conventionally called a **Schrödinger operator**.

Example 3.16 (Harmonic oscillator). Our main example for a system with non-zero potential is again the harmonic oscillator, $V = V_{\text{osc}} \geq 0$ from Example 3.8. In this case the Schrödinger operator $\hat{H} \geq 0$ may be defined by Friedrichs extension or form closure, Theorem 2.11, on $C_c^\infty(\mathbb{R}^d)$ and the form domain is

$$\mathcal{Q}(\hat{H}) = \mathcal{Q}(-\Delta) \cap \mathcal{Q}(V) = \left\{ \psi \in H^1(\mathbb{R}^d) : \int_{\mathbb{R}^d} |\mathbf{x}|^2 |\psi(\mathbf{x})|^2 d\mathbf{x} < \infty \right\}.$$

We note that $\{p_j, V(\mathbf{x})\} = -m\omega^2 x_j$, and hence one may take $\mathcal{O} = \text{Span}_{\mathbb{R}}\{1, x_j, p_k, H\}$ as a closed algebra of observables, with quantum representatives $\hat{\mathcal{O}} = \text{Span}_{\mathbb{R}}\{\mathbb{1}, \hat{x}_j, \hat{p}_k, \hat{H}\} \subseteq \mathcal{L}(\mathcal{H})$, all acting on a common dense domain $\mathcal{D}(\hat{H}) \subseteq \mathcal{Q}(\hat{H}) \subseteq \mathcal{H} = L^2(\mathbb{R}^d)$.

Alternatively, let us consider the closed algebra (3.8)-(3.9) spanned by $\{1, a_j, a_k^*, \mathcal{N}\}$ and try to quantize that. For simplicity we take $\hbar = 1$, $d = 1$ and drop the index $j = 1$. Note that $a \neq a^*$ (and also $a \neq -a^*$) since $\{a, a^*\} \neq 0$, and hence a or a^* are not observables. However, any of the expressions $aa^* = a^*a = \mathcal{N} = (a^*a + aa^*)/2 \in \mathcal{A}$ may be used. Also, given that we can extract from the real combinations $a + a^*$ and $-i(a - a^*)$ subject to (3.8) the original observables x resp. p and their canonical CCR, we may consider promoting a and a^* to *non-self-adjoint* operators \hat{a} resp. \hat{a}^* satisfying the commutation relations

$$[\hat{a}, \hat{a}^*] = \mathbb{1}, \quad [\hat{\mathcal{N}}, \hat{a}] = -\hat{a}, \quad [\hat{\mathcal{N}}, \hat{a}^*] = \hat{a}^*, \quad (3.31)$$

where we defined $\hat{\mathcal{N}} := \hat{a}^* \hat{a}$. Also note that $\hat{a} \hat{a}^* = \hat{\mathcal{N}} + \mathbb{1}$ by the first commutator above. Hence, the expressions that were the same on \mathcal{A} are now given by *different* operators. Furthermore, if we demand that $\hat{\mathcal{N}} = \hat{\mathcal{N}}^*$ is self-adjoint and has some non-trivial eigenstate $\psi \in \mathcal{H}$ with eigenvalue $\lambda \in \mathbb{R}$, then one may observe that $\hat{a}^k \psi$ resp. $(\hat{a}^*)^k \psi$ are also eigenstates with eigenvalues $\lambda - k$ resp. $\lambda + k$. Therefore, if also demanding $\hat{\mathcal{N}}$ to be bounded from below, there must exist a state $\psi_0 \in \mathcal{H}$ such that $\hat{a} \psi_0 = 0$, and the remaining states of an irreducible representation of (3.31) are then given by $\psi_k := (\hat{a}^*)^k \psi_0$ with $\hat{\mathcal{N}} \psi_k = k \psi_k$, $k = 0, 1, 2, \dots$ Taking finally the *symmetrized* expression $\hat{H}/\omega := (\hat{a}^* \hat{a} + \hat{a} \hat{a}^*)/2 = \hat{\mathcal{N}} + 1/2$, and $\mathcal{H} := \overline{\text{Span}\{\psi_k\}_{k=0}^\infty}$, this then provides the **algebraic solution** to the spectrum of the quantum Harmonic oscillator (one may finally show that these two representations coincide).

If V is unbounded from below then it is not certain that Friedrichs extension applies, but there are other tricks and concepts, such as relative form boundedness and relatively bounded perturbations, which may be used to define the sums of such forms and operators. However we will in this course rely solely on proving that the full Schrödinger expression (3.30) is bounded from below as a quadratic form, so that there is then an unambiguous choice of an associated bounded from below quantum Hamiltonian \hat{H} .

Example 3.17 (Coulomb potential). As already noted in Section 3.2, the Coulomb potential $V_C(\mathbf{x}) = -Z/|\mathbf{x}|$ is unbounded from below. In the next section we will use the uncertainty principle to prove that the form

$$q(\psi) := \left\langle \psi, \left[\frac{\hbar^2}{2m} (-\Delta_{\mathbb{R}^3}) - \frac{Z}{|\mathbf{x}|} \right] \psi \right\rangle$$

is nevertheless bounded from below on the minimal domain $C_c^\infty(\mathbb{R}^3)$ (also note here that, even though V_C is singular at $\mathbf{x} = \mathbf{0}$, we still have $V_C \in L_{\text{loc}}^1(\mathbb{R}^3)$ which makes the expression well defined on this domain), and hence it *defines* a semi-bounded from below self-adjoint operator \hat{H} by Theorem 2.11 or 2.12.

We remark that, as soon as we have defined a self-adjoint Hamiltonian operator \hat{H} which is bounded from below, $\hat{H} \geq -C$, then there cannot be any problems with the physical system for any future time, since all states $\psi \in \mathcal{H}$ then evolve unitarily by Stone's theorem, and furthermore arbitrarily negative values of the energy cannot be measured at any time since the measurable energy spectrum has a finite lower bound, $\sigma(\hat{H}) \subseteq [-C, +\infty)$. Hence, in this precise sense there is then **stability** for the corresponding quantum system.

Exercise 3.6. *Verify the algebraic relations in Example 3.16 and extend the solution to $d > 1$.*

Exercise 3.7. *Consider the angular momenta (3.29) in \mathbb{R}^3 , with L_1, L_2 and $L_3 := x_1 p_2 - x_2 p_1$ cyclically defined. Verify the Poisson brackets $\{L_1, L_2\} = L_3$ (cyclic) and $\{\mathbf{L}^2, L_k\} = 0$ for all k , where $\mathbf{L}^2 := L_1^2 + L_2^2 + L_3^2$. By considering $L_\pm := L_1 \pm iL_2$ and the corresponding commutation relations, show that all possible finite-dimensional irreducible quantizations of this algebra (with \hat{L}_k self-adjoint) may be labelled by a number $\ell \in \mathbb{Z}_{\geq 0}/2$ (called **spin**), and that the corresponding spectrum is $\sigma(\hat{L}_3) = \hbar\{-\ell, -\ell + 1, \dots, \ell\}$ and $\hat{\mathbf{L}}^2 = \hbar^2 \ell(\ell + 1)\mathbf{1}$.*

Exercise 3.8. *Show that $\hat{L}_j = \frac{1}{2}\sigma_j$ with the **Pauli matrices***

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

respectively $\hat{L}_j = iS_j$ the generators of rotations in \mathbb{R}^3 ,

$$S_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \quad S_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad S_3 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

yield irreducible representations of spin $\ell = 1/2$ resp. $\ell = 1$. Also note that \hat{L}_j^2 commute for these representations (is this always the case?).

3.5. The two-body problem and the hydrogenic atom. In the case that one considers *two* particles on \mathbb{R}^d , the classical configuration space would be $\mathcal{C}^{2d} = \mathbb{R}^d \times \mathbb{R}^d$ and the phase space $\mathcal{P}^{2d} = \mathbb{R}^{4d}$. We write the corresponding coordinates $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$ and momenta $\mathbf{p} = (\mathbf{p}_1, \mathbf{p}_2)$, with $\mathbf{x}_j, \mathbf{p}_k \in \mathbb{R}^d$. For the Hamiltonian, one could here think of adding the kinetic energies $T_j(\mathbf{p}_j) = \mathbf{p}_j^2/(2m_j)$ for each of the two particles $j = 1, 2$, and also allow for some potential on configuration space $V: \mathcal{C}^{2d} \rightarrow \mathbb{R}$ which depends on both particles:

$$H(\mathbf{x}, \mathbf{p}) = T_1(\mathbf{p}_1) + T_2(\mathbf{p}_2) + V(\mathbf{x}_1, \mathbf{x}_2) = \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + V(\mathbf{x}_1, \mathbf{x}_2) \quad (3.32)$$

Note that the masses m_1 resp. m_2 of the particles could be different, and that we may also w.l.o.g. rewrite the potential V into a sum of independent one-particle parts V_j and a final part W describing any **correlation** or **interaction** between the two particles,

$$V(\mathbf{x}_1, \mathbf{x}_2) = V_1(\mathbf{x}_1) + V_2(\mathbf{x}_2) + W(\mathbf{x}_1, \mathbf{x}_2),$$

thus

$$H(\mathbf{x}, \mathbf{p}) = \sum_{j=1,2} H_j(\mathbf{x}_j, \mathbf{p}_j) + W(\mathbf{x}_1, \mathbf{x}_2), \quad H_j(\mathbf{x}_j, \mathbf{p}_j) = \frac{\mathbf{p}_j^2}{2m_j} + V_j(\mathbf{x}_j).$$

In case there is no correlation between the particles, $W = 0$, this hence just describes a sum of two independent one-body Hamiltonians for which we may proceed with quantization as in Section 3.4. If we can find self-adjoint representations of the corresponding operators $\hat{H}_j \in \mathcal{L}(\mathfrak{H})$ on one-particle Hilbert spaces $\mathfrak{H} = L^2(\mathcal{C}^d) = L^2(\mathbb{R}^d)$ (the same \mathcal{C}^d for the two particles), then we can take the **two-body Hilbert space** to be the tensor product $\mathcal{H} = \mathfrak{H} \otimes \mathfrak{H} \cong L^2(\mathbb{R}^{2d})$ (see Exercise 3.9) and form a self-adjoint Hamiltonian operator out of two commuting ones:

$$\hat{H} = \hat{H}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \hat{H}_2 \in \mathcal{L}(\mathcal{H}), \quad \mathcal{D}(\hat{H}) = \mathcal{D}(\hat{H}_1) \otimes \mathcal{D}(\hat{H}_2),$$

with spectrum $\sigma(\hat{H}) = \overline{\sigma(\hat{H}_1) + \sigma(\hat{H}_2)}$ (see e.g. [Tes14, Section 4.6]). For brevity we will usually leave out the trivial factors of $\mathbb{1}$ in the tensor products if it is understood on which part of the space the operator acts. Also note that the expression for \hat{H} exponentiates to a unitary time evolution on **two-body states** $\Psi = \psi \otimes \phi \in \mathcal{H}$ (and linear combinations):

$$e^{it\hat{H}/\hbar}\Psi = (e^{it\hat{H}_1/\hbar} \otimes e^{it\hat{H}_2/\hbar})(\psi \otimes \phi) = e^{it\hat{H}_1/\hbar}\psi \otimes e^{it\hat{H}_2/\hbar}\phi.$$

Example 3.18. The d -dimensional harmonic oscillator from Example 3.16,

$$H(\mathbf{x}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{x}^2 = \sum_{j=1}^d \left(\frac{p_j^2}{2m} + \frac{1}{2}m\omega^2 x_j^2 \right),$$

separates into d copies of a one-dimensional oscillator, with no correlation between these different degrees of freedom, and hence it suffices to solve the one-dimensional problem to determine the full spectrum: $\sigma(\hat{H}) = \sum_{j=1}^d \omega(\mathbb{Z}_+ + 1/2) = \omega(\mathbb{Z}_+ + d/2)$.

In the case that there are correlations between the particles, $W \neq 0$, it may be helpful to change variables. For the Hamiltonian (3.32) we define the **center of mass** (COM) and its conjugate momentum

$$\mathbf{X} := \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1 + m_2}, \quad \mathbf{P} := \mathbf{p}_1 + \mathbf{p}_2, \quad (3.33)$$

as well as the **relative coordinate** with its conjugate momentum

$$\mathbf{r} := \mathbf{x}_1 - \mathbf{x}_2, \quad \mathbf{p}_r := \mu(\mathbf{p}_1/m_1 - \mathbf{p}_2/m_2). \quad (3.34)$$

Here

$$\mu := \frac{m_1 m_2}{m_1 + m_2}$$

is the **reduced mass** of the pair of particles. We may then rewrite the two-body Hamiltonian (3.32) in these coordinates as (see Exercise 3.10)

$$H(\mathbf{x}_1, \mathbf{x}_2; \mathbf{p}_1, \mathbf{p}_2) = \frac{\mathbf{P}^2}{2(m_1 + m_2)} + \frac{\mathbf{p}_r^2}{2\mu} + V\left(\mathbf{X} + \frac{\mu}{m_1}\mathbf{r}, \mathbf{X} - \frac{\mu}{m_2}\mathbf{r}\right) =: \tilde{H}(\mathbf{X}, \mathbf{r}; \mathbf{P}, \mathbf{p}_r).$$

Example 3.19 (The hydrogenic atom). Recall from Section 3.2 that the hydrogenic atom consists of a nucleus with charge $Z > 0$ and an electron with charge -1 , which interact via the Coulomb potential $V_C(\mathbf{r}) = -Z/|\mathbf{r}|$, where $|\mathbf{r}|$ is the distance between the particles in

\mathbb{R}^3 . The proper model is therefore a two-body classical configuration space $\mathcal{C}^{3 \times 2} = \mathbb{R}^3 \times \mathbb{R}^3$, phase space $\mathcal{P}^{3 \times 2} = \mathbb{R}^{12}$, and Hamiltonian

$$H(\mathbf{x}_1, \mathbf{x}_2; \mathbf{p}_1, \mathbf{p}_2) = \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} - \frac{Z}{|\mathbf{x}_1 - \mathbf{x}_2|},$$

with m_1 and m_2 the masses of the nucleus and electron, respectively. It is here appropriate to switch to COM and relative coordinates, $\mathcal{C}^{3 \times 2} \cong \mathcal{C}_{\text{cm}} \times \mathcal{C}_{\text{rel}} \ni (\mathbf{X}, \mathbf{r})$, in which the Hamiltonian separates,

$$\tilde{H}(\mathbf{X}, \mathbf{r}; \mathbf{P}, \mathbf{p}_r) = \frac{\mathbf{P}^2}{2(m_1 + m_2)} + \frac{\mathbf{p}_r^2}{2\mu} - \frac{Z}{|\mathbf{r}|}.$$

The first term involving the center-of-mass momentum \mathbf{P} is just the one-body Hamiltonian $H_{\text{cm}}(\mathbf{X}; \mathbf{P})$ of a free particle on $\mathcal{C}_{\text{cm}} = \mathbb{R}^3$, which we may quantize uniquely along the lines of Example 3.15, while the second two terms constitute the Hamiltonian $H_{\text{rel}}(\mathbf{r}; \mathbf{p}_r)$ of the one-body Coulomb problem on $\mathcal{C}_{\text{rel}} = \mathbb{R}^3$ which was discussed classically in Section 3.2 and quantum-mechanically in Example 3.17 of Section 3.4, and which we shall return to many more times. Given a self-adjoint quantization $\hat{H}_{\text{rel}} \in \mathcal{L}(L^2(\mathcal{C}_{\text{rel}}))$ of this Hamiltonian, we therefore have the two-particle operator

$$\hat{H} = \frac{\hbar^2(-\Delta_{\mathbf{X}})}{2(m_1 + m_2)} \otimes \mathbf{1} + \mathbf{1} \otimes \hat{H}_{\text{rel}}, \quad \mathcal{D}(\hat{H}) = H^2(\mathbb{R}^3) \otimes \mathcal{D}(\hat{H}_{\text{rel}}),$$

on the two-particle quantum configuration space $\mathcal{H} = L^2(\mathbb{R}^3, d\mathbf{X}) \otimes L^2(\mathbb{R}^3, d\mathbf{r})$. Again then,

$$\sigma(\hat{H}) = \overline{\sigma(\hat{H}_{\text{cm}})} + \overline{\sigma(\hat{H}_{\text{rel}})} = [0, \infty) + \sigma(\hat{H}_{\text{rel}}) = [\inf \sigma(\hat{H}_{\text{rel}}), \infty),$$

and we see that the spectrum of the free center-of-mass motion in the end obscures most of the information about the relative one. Therefore, in practice one often removes the COM part from the problem altogether and then studies only the more interesting relative part.

Exercise 3.9. Use Fubini's theorem to show that $L^2(X, \mu) \otimes L^2(Y, \nu) \cong L^2(X \times Y, \mu \times \nu)$, where μ, ν are σ -finite measures and, for two Hilbert spaces \mathcal{H}, \mathcal{K} , $\mathcal{H} \otimes \mathcal{K}$ is defined with

$$\langle u_1 \otimes u_2, v_1 \otimes v_2 \rangle_{\mathcal{H} \otimes \mathcal{K}} := \langle u_1, v_1 \rangle_{\mathcal{H}} \langle u_2, v_2 \rangle_{\mathcal{K}}.$$

Exercise 3.10. Verify that the COM and relative coordinates and momenta (3.33)-(3.34) are canonically conjugate, i.e

$$\{(\mathbf{X})_j, (\mathbf{P})_k\} = \delta_{jk}, \quad \{(\mathbf{r})_j, (\mathbf{p}_r)_k\} = \delta_{jk},$$

and all other Poisson brackets in $\mathbf{X}, \mathbf{r}, \mathbf{P}$ and \mathbf{p}_r are zero, and furthermore that

$$m_1 \mathbf{x}_1^2 + m_2 \mathbf{x}_2^2 = (m_1 + m_2) \mathbf{X}^2 + \mu \mathbf{r}^2, \quad \frac{\mathbf{p}_1^2}{m_1} + \frac{\mathbf{p}_2^2}{m_2} = \frac{\mathbf{P}^2}{m_1 + m_2} + \frac{\mathbf{p}_r^2}{\mu}.$$

3.6. The N -body problem. We may extend much of the above analysis to the N -body problem, that is, we may consider N particles on \mathbb{R}^d with masses m_j and with independent one-body potentials $V_j(\mathbf{x}_j)$, two-body correlation potentials $W_{jk}(\mathbf{x}_j, \mathbf{x}_k)$ describing pairwise interactions between particles \mathbf{x}_j and \mathbf{x}_k with $j \neq k$, as well as three-body interactions $W_{jkl}(\mathbf{x}_j, \mathbf{x}_k, \mathbf{x}_l)$ with j, k, l all distinct, and so on. Although interaction potentials involving more than two particles are not uncommon in physics, they will not be relevant for our stability of matter problem and shall hence for simplicity not be considered further in this course (except perhaps occasionally). Furthermore, it is common that the one-body

potentials have already incorporated all the dependence on absolute positions such as pair-wise centers of mass, and hence that the pair-interactions W_{jk} are translation-invariant, i.e., depending only on the relative coordinate $\mathbf{r}_{jk} := \mathbf{x}_j - \mathbf{x}_k$ of each pair (w.l.o.g. $j < k$).

With these restrictions or simplifications, the **N -body Hamiltonian** on the classical configuration space $\mathcal{C}^{d \times N} = (\mathbb{R}^d)^N$ and phase space $\mathcal{P}^{d \times N} = (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$ may thus be defined

$$H(\mathbf{x}, \mathbf{p}) := \sum_{j=1}^N (T_j(\mathbf{p}_j) + V_j(\mathbf{x}_j)) + \sum_{1 \leq j < k \leq N} W_{jk}(\mathbf{x}_j - \mathbf{x}_k) = T(\mathbf{p}) + V(\mathbf{x}) + W(\mathbf{x}).$$

Again we see that there is no ordering ambiguity here since the terms involve coordinates and momenta separately. The natural quantum version of the expression is therefore

$$\hat{H} := \sum_{j=1}^N (T_j(\hat{\mathbf{p}}_j) + V_j(\hat{\mathbf{x}}_j)) + \sum_{1 \leq j < k \leq N} W_{jk}(\hat{\mathbf{x}}_j - \hat{\mathbf{x}}_k) = \hat{T} + \hat{V} + \hat{W},$$

which is to be acting as an operator on $\mathcal{H} = L^2(\mathcal{C}^{d \times N}) = L^2(\mathbb{R}^{dN})$, that is, we should try to implement these expressions as operators or forms on some space \mathcal{F} of sufficiently well-behaved functions $\Psi \in L^2(\mathcal{C}^{d \times N})$, called **N -body quantum states** or **N -body wave functions**, according to

$$\begin{aligned} \hat{T}\Psi(\mathbf{x}) &:= \sum_{j=1}^N \frac{\hat{\mathbf{p}}_j^2}{2m_j} \Psi(\mathbf{x}) = - \sum_{j=1}^N \frac{\hbar^2}{2m_j} \Delta_{\mathbf{x}_j} \Psi(\mathbf{x}), \\ \hat{V}\Psi(\mathbf{x}) &:= \sum_{j=1}^N V_j(\mathbf{x}_j) \Psi(\mathbf{x}), \\ \hat{W}\Psi(\mathbf{x}) &:= \sum_{1 \leq j < k \leq N} W_{jk}(\mathbf{x}_j - \mathbf{x}_k) \Psi(\mathbf{x}). \end{aligned} \tag{3.35}$$

Which space \mathcal{F} we may choose depends on details of the potentials V and W , namely, if for example the interaction W is too singular then this may force us to consider only those functions which vanish (sufficiently fast) at the singularities. Hence, the usual minimal domain $C_c^\infty(\mathbb{R}^{dN}) \subseteq \mathcal{H}$ might not always be appropriate, as the following example illustrates.

Example 3.20 (Hard-core interaction). Consider an interaction potential $W_R(\mathbf{r})$ formally defined by

$$W_R(\mathbf{r}) = \begin{cases} +\infty, & \text{if } |\mathbf{r}| < R, \\ 0, & \text{if } |\mathbf{r}| \geq R. \end{cases}$$

This describes **hard spheres** (or **hard cores**) of radius $R/2$, because as soon as the particles are within a distance $|\mathbf{r}| = |\mathbf{x}_j - \mathbf{x}_k| < R$ the energy is infinite — a very hard collision — and otherwise they do not see each other. Since the corresponding form on the relative Hilbert space $L^2(\mathbb{R}^d, d\mathbf{r})$ is formally

$$\langle \psi, W_R \psi \rangle = \int_{\mathbb{R}^d} W_R |\psi|^2 = \begin{cases} +\infty, & \text{if } |B_R(0) \cap \text{supp } \psi| > 0, \\ 0, & \text{otherwise,} \end{cases}$$

the mathematically precise way to incorporate this potential is to consider a *new* minimal domain $\mathcal{D}(W_R) = C_c^\infty(B_R(0)^c) \subseteq \mathcal{H}$ and a corresponding restriction in the Hilbert space

$\mathcal{H} = L^2(B_R(0)^c) = \overline{\mathcal{D}(W_R)}$ (the closure may be taken in the old Hilbert space $L^2(\mathbb{R}^d)$). This enforces the knowledge that there is zero probability that the particles overlap.

Note that (again by Exercise 3.9) we may equivalently think of $\Psi \in L^2(\mathbb{R}^{dN}) \cong \otimes^N \mathfrak{H}$ as tensor products (including any finite linear combinations and limits thereof) of one-particle states $\psi_n \in \mathfrak{H} = L^2(\mathbb{R}^d)$,

$$\Psi = \sum_{n_1=1}^{\infty} \cdots \sum_{n_N=1}^{\infty} c_{n_1 \dots n_N} \psi_{n_1} \otimes \cdots \otimes \psi_{n_N}, \quad c_{n_1 \dots n_N} \in \mathbb{C}.$$

In the case that all $W_{jk} = 0$ we again have a separation of the problem into independent one-body problems,

$$\hat{H} = \sum_{j=1}^N \hat{h}_j, \quad \hat{h}_j = -\frac{\hbar^2}{2m_j} \Delta_{\mathbf{x}_j} + V_j(\mathbf{x}_j) \in \mathcal{L}(\mathfrak{H}), \quad (3.36)$$

and, if these are subsequently realized as self-adjoint operators, then $\sigma(\hat{H}) = \overline{\sum_{j=1}^N \sigma(\hat{h}_j)}$.

Also, if $W_{jk} \neq 0$, then one may for each pair of particles instead consider the problem in the corresponding relative coordinates \mathbf{r}_{jk} . However, because for $N > 2$ there are more pairs than relative degrees of freedom, $\binom{N}{2} > N - 1$, this forms a redundant set of variables and the problem typically does not separate. The total center of mass,

$$\mathbf{X} = \sum_{j=1}^N m_j \mathbf{x}_j / \sum_{j=1}^N m_j, \quad \mathbf{P} = \sum_{j=1}^N \mathbf{p}_j,$$

may still be separated away though if the one-body potential V admits such a separation. We will not consider the appropriate change of variables in the general case, involving **Jacobi coordinates**, but only in the below special case of identical masses.

3.6.1. Models of matter and notions of stability. An important special case is that all the particles are of exactly the same kind so that we have the same mass $m_j = m$ and one-particle interaction $V_j = V$ for all j , and also that the two-particle interaction $W_{jk} = W$ is independent of the pair considered and furthermore symmetric w.r.t. particle exchange $\mathbf{r}_{jk} \mapsto -\mathbf{r}_{jk} = \mathbf{r}_{kj}$, i.e. $W(\mathbf{r}_{jk}) = W(-\mathbf{r}_{jk})$. The resulting Hamiltonian operator

$$\hat{H}^N := \sum_{j=1}^N \left(\frac{\hbar^2}{2m} (-\Delta_{\mathbf{x}_j}) + V(\mathbf{x}_j) \right) + \sum_{1 \leq j < k \leq N} W(\mathbf{x}_j - \mathbf{x}_k) \quad (3.37)$$

then defines the **typical N -body quantum system** involving a single type of particle.

In this case it may be useful to write the momenta as a sum of pairs using the **generalized parallelogram identity** (valid on \mathbb{C}^d or general Hilbert spaces; cf. Example 2.3),

$$\sum_{j=1}^N |\mathbf{p}_j|^2 = \frac{1}{N} \left| \sum_{j=1}^N \mathbf{p}_j \right|^2 + \frac{1}{N} \sum_{1 \leq j < k \leq N} |\mathbf{p}_j - \mathbf{p}_k|^2, \quad (3.38)$$

and thus for the Hamiltonian

$$\hat{H}^N = \frac{\hbar^2}{2mN} (-\Delta_{\mathbf{X}}) + \sum_{1 \leq j < k \leq N} \left(\frac{1}{2mN} |\hat{\mathbf{p}}_j - \hat{\mathbf{p}}_k|^2 + \frac{1}{N-1} (V(\mathbf{x}_j) + V(\mathbf{x}_k)) + W(\mathbf{r}_{jk}) \right).$$

Again, although it looks as if we may have separated the problem if $V = 0$, this is indeed true for the COM variable but the particle pairs are actually *not* independent.

Another important case will in fact constitute our **model of matter** in the sequel. Here we have *two* species of particles: N electrons and M nuclei, with positions $\mathbf{x}_j \in \mathbb{R}^d$ respectively $\mathbf{R}_k \in \mathbb{R}^d$. The quantum Hamiltonian on $L^2(\mathcal{C}^{d \times N} \times \mathcal{C}^{d \times M})$ is

$$\hat{H}^{N,M} := \sum_{j=1}^N \frac{\hbar^2}{2m_e} (-\Delta_{\mathbf{x}_j}) + \sum_{k=1}^M \frac{\hbar^2}{2m_n} (-\Delta_{\mathbf{R}_k}) + W_C(\mathbf{x}, \mathbf{R}), \quad (3.39)$$

with masses $m_e > 0$ respectively $m_n > 0$, and where we have taken as the interaction the (N, M) -**body Coulomb potential**:

$$W_C(\mathbf{x}, \mathbf{R}) := \sum_{1 \leq i < j \leq N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} - \sum_{j=1}^N \sum_{k=1}^M \frac{Z}{|\mathbf{x}_j - \mathbf{R}_k|} + \sum_{1 \leq k < l \leq M} \frac{Z^2}{|\mathbf{R}_k - \mathbf{R}_l|} \quad (3.40)$$

This implements the appropriate Coulomb interaction (3.11) between each pair of particles, where the charges are again $q_e = -1$ for the electrons and $q_n = Z > 0$ for the nuclei. One may also add external one-body potentials V_e respectively V_n , although we will not do so here but rather consider the whole system (3.39) of $N + M$ particles to be completely *free* apart from the internal interactions in W_C . Sometimes we may however consider the kinetic energies of the nuclei to be irrelevant for the problem since in reality $m_n \gg m_e$ and thus we could consider this as a limit $m_n \rightarrow \infty$. We may in any case drop the non-negative terms $(-\Delta_{\mathbf{R}_k})/(2m_n) \geq 0$ for a lower bound to $\hat{H}^{N,M}$. Upon doing so the positions $\mathbf{R} = (\mathbf{R}_1, \dots, \mathbf{R}_M)$ of the nuclei remain as parameters of the resulting N -body Hamiltonian $\hat{H}^N(\mathbf{R})$ and the corresponding terms of the interaction W_C are then treated as external one-body potentials.

Definition 3.21 (Ground-state energy, and stability of the first and second kind). Given a quantum system modeled on a Hilbert space \mathcal{H} with a self-adjoint Hamiltonian operator $\hat{H} \in \mathcal{L}(\mathcal{H})$, we define its **ground-state energy** to be the infimum of the spectrum,

$$E_0 := \inf \sigma(\hat{H}) = \inf_{\psi \in \mathcal{Q}(\hat{H}) \setminus \{0\}} \left\langle \hat{H} \right\rangle_{\psi}.$$

We say that the system is **stable of the first kind** iff \hat{H} is bounded from below,

$$E_0 > -\infty.$$

Moreover, in the case that the system depends on a total of N particles, with $\mathcal{H} = \mathcal{H}^N$, $\hat{H} = \hat{H}^N$, and

$$E_0(N) := \inf \sigma(\hat{H}^N) = \inf_{\Psi \in \mathcal{Q}(\hat{H}^N) \setminus \{0\}} \left\langle \hat{H}^N \right\rangle_{\Psi},$$

then it is called **stable of the second kind** iff \hat{H}^N admits a lower bound which is at most *linearly* divergent in N , i.e. iff there exists a constant $C \geq 0$ such that for all $N \in \mathbb{N}$

$$E_0(N) \geq -CN.$$

Remark 3.22. A stable system does not necessarily have a **ground state**, i.e. some eigenstate $\psi \in \mathcal{H} \setminus \{0\}$ with energy equal to the ground-state energy E_0 , $\hat{H}\psi = E_0\psi$. For example the free particle on \mathbb{R}^d (Example 3.15) is certainly stable with $E_0 = 0$ but has no ground

state, since the only sensible candidate would be either the constant function (in the usual form sense, $\langle \psi, -\Delta\psi \rangle = \|\nabla\psi\|^2 = 0$) or perhaps a harmonic function (in the operator sense, $-\Delta\psi = 0$) which in either case is not in $L^2(\mathbb{R}^d)$.

3.6.2. Density and particle probabilities. The problem with the models of matter (3.37) and (3.39) is that it is in practice *extremely* difficult to compute their spectra $\sigma(\hat{H})$, even numerically on any foreseeable supercomputer, since in reality N is typically extremely large. In just 1 gram of matter there are $N \sim 10^{23}$ particles (and, in fact, even the classical many-body problem is then almost impossible to understand on the individual particle level). The approach one takes instead is to try to reduce this problem, which takes place on the enormous classical configuration space \mathbb{R}^{dN} with $N \gg 1$, to an approximate problem on some space of fixed small dimension such as \mathbb{R}^d .

Recall that if Ψ is normalized in $L^2(\mathbb{R}^{dN})$ — which we shall assume from now on for our quantum states — then $|\Psi(\mathbf{x})|^2$ may be interpreted as the probability density of finding the particles at positions $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_N) \in (\mathbb{R}^d)^N$. We may however instead define a corresponding particle density on the one-body configuration space \mathbb{R}^d :

Definition 3.23 (One-body density). The **one-body density** associated to a *normalized* N -body wave function $\Psi \in L^2((\mathbb{R}^d)^N)$ is the function $\varrho_\Psi \in L^1(\mathbb{R}^d)$ given by

$$\varrho_\Psi(\mathbf{x}) := \sum_{j=1}^N \int_{\mathbb{R}^{d(N-1)}} |\Psi(\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{x}, \mathbf{x}_{j+1}, \dots, \mathbf{x}_N)|^2 \prod_{k \neq j} d\mathbf{x}_k. \quad (3.41)$$

The interpretation of this expression is that it is a sum of contributions to a particle density, where each term gives the probability of finding particle j at $\mathbf{x} \in \mathbb{R}^d$ while all the other particles are allowed to be anywhere in \mathbb{R}^d and hence with their positions integrated out. Because of the sum, we have no information in $\varrho_\Psi(\mathbf{x})$ which one of the N particles was at \mathbf{x} but only how many were there on average. Indeed, $\int_\Omega \varrho_\Psi$ will be the expected number of particles to be found on the set $\Omega \subseteq \mathbb{R}^d$, and we can write

$$\int_\Omega \varrho_\Psi = \left\langle \sum_{j=1}^N \mathbb{1}_{\{\mathbf{x}_j \in \Omega\}} \right\rangle_\Psi \quad \text{and} \quad \varrho_\Psi(\mathbf{x}) = \left\langle \sum_{j=1}^N \delta_{\mathbf{x}_j = \mathbf{x}} \right\rangle_\Psi$$

in accordance with the interpretations of Remark 3.11.2 and Section 3.3.2. Note that $\int_{\mathbb{R}^d} \varrho_\Psi = N$ since every particle has to be somewhere in \mathbb{R}^d .

Further note that using ϱ_Ψ we can now write for the expectation value of the one-body potential

$$\langle \hat{V} \rangle_\Psi = \int_{\mathbb{R}^d} V(\mathbf{x}) \varrho_\Psi(\mathbf{x}) d\mathbf{x},$$

which is indeed a tremendous simplification of the full N -body form to only depend on the one-body density. Unfortunately a similar straightforward simplification does not occur for the kinetic and interaction energies $\langle \hat{T} \rangle_\Psi$ and $\langle \hat{W} \rangle_\Psi$, and the task of physicists and mathematicians working in many-body quantum theory is to try to find such simplifications. We shall come across some important instances of this later in the course.

We will also find it useful to extract the **local particle probability distribution** encoded in the full wave function Ψ . Namely, given a subset $\Omega \subseteq \mathbb{R}^d$ of the one-body configuration space and a subset $A \subseteq \{1, 2, \dots, N\}$ of the particles (particle labels), we may

form the probability to find *exactly* those particles on Ω and the rest outside Ω (i.e. on its complement $\Omega^c = \mathbb{R}^d \setminus \Omega$):

$$p_{A,\Omega}[\Psi] := \left\langle \prod_{k \in A} \mathbb{1}_{\{\mathbf{x}_k \in \Omega\}} \prod_{k \notin A} \mathbb{1}_{\{\mathbf{x}_k \in \Omega^c\}} \right\rangle_{\Psi} = \int_{(\Omega^c)^{N-|A|}} \int_{\Omega^{|A|}} |\Psi|^2 \prod_{k \in A} d\mathbf{x}_k \prod_{k \notin A} d\mathbf{x}_k.$$

The probability of finding exactly n particles on Ω *irrespective of their labels* is then the sum of all such possibilities

$$p_{n,\Omega}[\Psi] := \sum_{A \subseteq \{1, \dots, N\} \text{ s.t. } |A| = n} p_{A,\Omega}[\Psi].$$

We then note that (exercise)

$$\sum_{n=0}^N p_{n,\Omega}[\Psi] = \sum_{A \subseteq \{1, \dots, N\}} p_{A,\Omega}[\Psi] = \int_{\mathbb{R}^{dN}} |\Psi|^2 = 1, \quad (3.42)$$

in other words, some number of particles (possibly zero) and some subset of the particles (possibly the empty one) must always be found on Ω . Also, the **expected number of particles** to be found on Ω is (exercise)

$$\sum_{n=0}^N n p_{n,\Omega}[\Psi] = \sum_{j=1}^N \int_{\mathbb{R}^{dN}} \mathbb{1}_{\Omega}(\mathbf{x}_j) |\Psi(\mathbf{x})|^2 dx = \int_{\Omega} \varrho_{\Psi}, \quad (3.43)$$

which agrees with our earlier interpretations.

Remark 3.24. There is also a more general concept of **density matrices**, which certainly is very useful but will not be treated here. We refer instead to e.g. [LS10, Chapter 3.1.4].

Remark 3.25 (Fock spaces). For settings where the number N of particles can vary with time it is necessary to introduce an appropriate space containing all different particle numbers, known as a **Fock space**:

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{H}^N = \mathbb{C} \oplus \mathfrak{H} \oplus \mathcal{H}^2 \oplus \dots$$

where $\mathcal{H}^N = \otimes^N \mathfrak{H}$ is the N -body space. The concept will not be applied in this course however, as we will only be working with time-independent Hamiltonians with a fixed number of particles.

Exercise 3.11. Prove (3.38) for arbitrary $\mathbf{p}_j \in \mathbb{C}$.

Exercise 3.12. Prove (3.42) and (3.43) by inserting and expanding the identity

$$\mathbb{1} = \prod_{k=1}^N (\mathbb{1}_{\Omega}(\mathbf{x}_k) + \mathbb{1}_{\Omega^c}(\mathbf{x}_k)) = \sum_{A \subseteq \{1, 2, \dots, N\}} \mathbb{1}_{\mathbf{x}_k \in A \in \Omega} \mathbb{1}_{\mathbf{x}_k \notin A \in \Omega^c}. \quad (3.44)$$

3.7. Identical particles and quantum statistics. It will turn out that our model of matter (3.39) as presently formulated is actually *unstable* with $N + M \rightarrow \infty$. Although it is very hard to see it directly in (3.39)–(3.40) — and indeed we have not yet even settled stability for the hydrogen atom $N = M = 1$, the topic of the next section — a picture one could keep in mind for now is that of a single massive atom with a large nucleus (or charge $Z \gg 1$) surrounded by many electrons (say $N = Z$ to make the system neutral). If we may ignore their mutual Coulomb repulsion, these electrons would all prefer to sit in the tightest orbit with the lowest energy, and this turns out to diverge too fast with N for stability. You could at this stage think of the atom’s energy levels as similar to the harmonic oscillator energy levels, although in the attractive Coulomb potential of the nucleus they will be negative and accumulating to zero, with the lowest level proportional to $-Z^2 \sim -N^2$, yielding a total energy $\sim -N^3$ for the electrons. However, this picture turns out not to be the correct one, not simply because of the neglected Coulomb repulsion terms, but perhaps more importantly because of an additional *fundamental* property of electrons which was not visible classically. Namely, apart from the uncertainty principle arising as a consequence of the non-commutativity relations of operator observables, an additional pair of intimately related and fundamentally new concepts brought in by quantum mechanics is that of **identical particles** and **quantum statistics**.

We have already assumed in (3.37) and (3.39) that all N (or M) particles are of the same kind, for example electrons, which means that they all have the exact same physical properties such as mass and charge, and therefore behave in the exact same way. In fact no measurement can ever distinguish one such particle from another. In quantum mechanics, where the uncertainty principle sets fundamental (logical) limits to distinguishability, this becomes a very important logical distinction since the particles must therefore be treated as **logically identical**. In particular, considering the probability density of an N -body state $\Psi \in L^2((\mathbb{R}^d)^N)$ of such **indistinguishable particles**, we must have a symmetry upon exchanging two particles j and k ,

$$|\Psi(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_k, \dots, \mathbf{x}_N)|^2 = |\Psi(\mathbf{x}_1, \dots, \mathbf{x}_k, \dots, \mathbf{x}_j, \dots, \mathbf{x}_N)|^2, \quad j \neq k, \quad (3.45)$$

since we cannot tell which one is which. However, since Ψ takes values in \mathbb{C} , this relation involving only the amplitude would still allow for a phase difference,

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_k, \dots, \mathbf{x}_N) = e^{i\theta_{jk}} \Psi(\mathbf{x}_1, \dots, \mathbf{x}_k, \dots, \mathbf{x}_j, \dots, \mathbf{x}_N), \quad j \neq k. \quad (3.46)$$

One may then argue that a double exchange does nothing to the state (the square of a transposition is the identity) so we must have $(e^{i\theta_{jk}})^2 = 1$, that is $\theta_{jk} = 0$ or π . Further, by considering the expectation values of symmetric N -particle operator observables (see [MG64, Gir65, Gir69] for a more elaborate argument, as well as Exercise 3.13) one may also realize that, for consistency, these phases cannot depend on which pair is considered, i.e. on j or k . The only possibility is then that Ψ satisfies either

$$\Psi(\mathbf{x}_{\sigma(1)}, \mathbf{x}_{\sigma(2)}, \dots, \mathbf{x}_{\sigma(N)}) = \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \dots, \mathbf{x}_N), \quad (3.47)$$

for any permutation $\sigma \in S_N$ of the indices, in which case we refer to these N identical particles as **bosons**, or

$$\Psi(\mathbf{x}_{\sigma(1)}, \mathbf{x}_{\sigma(2)}, \dots, \mathbf{x}_{\sigma(N)}) = \text{sign}(\sigma) \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \dots, \mathbf{x}_N), \quad (3.48)$$

for which the particles are instead called **fermions**. Hence, this amounts to a reduction of the full Hilbert space $\mathcal{H} = L^2(\mathbb{R}^{dN}) \cong \otimes^N \mathfrak{H}$, $\mathfrak{H} = L^2(\mathbb{R}^d)$, of (distinguishable) N -body

quantum states into the *symmetric* subspace

$$\mathcal{H}_{\text{sym}} = L^2_{\text{sym}}((\mathbb{R}^d)^N) := \{\Psi \in L^2(\mathbb{R}^{dN}) : \Psi \text{ satisfies (3.47)} \forall \sigma \in S_N\} \cong \bigotimes_{\text{sym}}^N \mathfrak{H},$$

or the *antisymmetric* subspace

$$\mathcal{H}_{\text{asym}} = L^2_{\text{asym}}((\mathbb{R}^d)^N) := \{\Psi \in L^2(\mathbb{R}^{dN}) : \Psi \text{ satisfies (3.48)} \forall \sigma \in S_N\} \cong \bigwedge^N \mathfrak{H}.$$

The above argument to fix the phase ambiguity (3.46) of Ψ under particle exchange was the standard one in the first half of a century after the discovery of quantum mechanics, and is in fact still today commonly applied in physics textbooks without further discussion. However, in the 1970's it was clarified (see [LM77], or e.g. [Myr99] for review⁽¹³⁾) that this is actually not the complete appropriate way to think about the problem for identical particles. Rather, even *before* quantization, the *classical* configuration space $\mathcal{C}^{d \times N} = \mathbb{R}^{dN}$ should be replaced by the *symmetrized* one

$$\mathcal{C}_{\text{sym}}^{d \times N} := \left((\mathbb{R}^d)^N \setminus \Delta \right) / S_N,$$

simply because there is no way to distinguish the particles even classically. Here we have first removed the set of particle coincidences⁽¹⁴⁾, i.e. the **fat diagonal**⁽¹⁵⁾ of the configuration space

$$\Delta := \{(\mathbf{x}_1, \dots, \mathbf{x}_N) \in (\mathbb{R}^d)^N : \exists j \neq k \text{ s.t. } \mathbf{x}_j = \mathbf{x}_k\}, \quad (3.49)$$

and then taken the quotient under the action of the group S_N of permutations of N indices,

$$\sigma : (\mathbf{x}_1, \dots, \mathbf{x}_N) \mapsto (\mathbf{x}_{\sigma(1)}, \mathbf{x}_{\sigma(2)}, \dots, \mathbf{x}_{\sigma(N)}),$$

to obtain the set of **proper N -point subsets** of \mathbb{R}^d :

$$\mathcal{C}_{\text{sym}}^{d \times N} = \{A = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subseteq \mathbb{R}^d : |A| = N\}.$$

This is the natural space of configurations for N truly indistinguishable (logically identical) particles, and while it changes very little on the classical side, e.g. only marginally the space where one may define potentials $V(\mathbf{x})$ since they anyway have to be symmetric under permutations, it does affect the possible quantizations of the free kinetic energy $T(\mathbf{p}) = (2m)^{-1}|\mathbf{p}|^2$, which turn out to depend on the non-trivial *topology* of this configuration space. In particular, particle exchange no longer makes sense as a permutation of indices (note that this is the identity operation on the quotient $\mathcal{C}_{\text{sym}}^{d \times N}$) but should instead be considered as a *continuous* operation which relates points in the configuration space via paths. The consequences of this approach have by now been studied in detail and are quite well understood even on a strict mathematical level (although some important questions still remain open). To give the full story would be a course in itself, however, and we will only state the main points here, guided by the following simpler example:

⁽¹³⁾Note however that there were plenty of earlier hints, and the story actually goes back all the way to Gibbs' classical statistical mechanics; see e.g. [Frö90] and references therein, as well as [Gir65][Sou70, p. 386].

⁽¹⁴⁾This can be motivated by the fact that if some positions exactly coincide then we cannot tell if there really are N particles, which is what we want to consider here. It may also be justified a posteriori [BS92].

⁽¹⁵⁾The *thin* diagonal would be the points $\mathbf{x} \in \mathbb{R}^{dN}$ such that $\mathbf{x}_1 = \mathbf{x}_2 = \dots = \mathbf{x}_N$.

Example 3.26 (Two identical particles). Consider just one pair of particles on \mathbb{R}^d whose configuration space in the distinguishable case is $\mathcal{C}^{d \times 2} = \mathbb{R}^d \times \mathbb{R}^d \ni (\mathbf{x}_1, \mathbf{x}_2)$, while the indistinguishable one is

$$\mathcal{C}_{\text{sym}}^{d \times 2} = \left(\mathbb{R}^d \times \mathbb{R}^d \setminus \Delta \right) / \sim, \quad \Delta = \{(\mathbf{x}, \mathbf{x}) : \mathbf{x} \in \mathbb{R}^d\},$$

with the identification $(\mathbf{x}_1, \mathbf{x}_2) \sim (\mathbf{x}_2, \mathbf{x}_1)$ of the particles. The geometry of this space becomes more transparent upon changing to COM and relative coordinates, $(\mathbf{X}, \mathbf{r}) \in \mathcal{C}_{\text{cm}} \times \mathcal{C}_{\text{rel}}$. The space then separates into $\mathcal{C}_{(\text{sym})}^{d \times 2} \cong \mathcal{C}_{\text{cm}} \times \mathcal{C}_{\text{rel}}^{(\text{sym})}$ where $\mathcal{C}_{\text{cm}} = \mathbb{R}^d$, and the relative space in the distinguishable case is $\mathcal{C}_{\text{rel}} = \mathbb{R}^d$ while in the indistinguishable case it is $\mathcal{C}_{\text{rel}}^{\text{sym}} = (\mathbb{R}^d \setminus \{0\}) / \sim$ with the antipodal identification $\mathbf{r} \sim -\mathbf{r}$. The diagonal $\Delta \cong \mathcal{C}_{\text{cm}} \times \{0\}$ corresponds precisely to $\mathbf{r} = 0$. The remaining relative space may finally be parameterized in terms of the pairwise distance $r > 0$ and a relative angle $\omega \in \mathbb{S}^{d-1}$ or $\omega \in \mathbb{S}^{d-1} / \sim$.

Note that the topology of $\mathcal{C}_{\text{rel}}^{\text{sym}}$ varies markedly with dimension, namely consider the fundamental group π_1 of this topological space:

$$\pi_1(\mathcal{C}_{\text{rel}}^{\text{sym}}) \cong \pi_1(\mathbb{S}^{d-1} / \sim) = \begin{cases} \pi_1(\mathbb{R}P^{d-1}) \cong \mathbb{Z}_2, & d \geq 3, \\ \pi_1(\mathbb{S}^1) \cong \mathbb{Z}, & d = 2, \\ \pi_1(\{1\}) \cong 1, & d = 1. \end{cases}$$

The group π_1 is by definition the group of continuous loops⁽¹⁶⁾ in the space modulo continuous deformations (homotopy equivalences), and it is exactly this group which describes the non-trivial *continuous* particle exchanges, amounting to continuous loops or particle trajectories $\gamma \subset \mathcal{C}_{\text{rel}}^{\text{sym}}$ modulo any such loops that are topologically trivial (trivial in this sense means that no exchange has taken place, the particles may just have wiggled a bit).

In the case $d = 1$ we have $\mathcal{C}_{\text{rel}}^{\text{sym}} \cong \mathbb{R}^+$ and the group of loops is trivial, while for $d = 2$ and $\mathbb{S}^1 / \sim \cong \mathbb{S}^1$ the generator τ of the group $\pi_1(\mathcal{C}_{\text{rel}}^{\text{sym}}) \cong \pi_1(\mathbb{S}^1)$ may be chosen as a *simple* (say counter-clockwise) loop, and an arbitrary element is $[\gamma] = \tau^n$, $n \in \mathbb{Z}$ the **winding number** of the loop. In the case $d \geq 3$ one finds by an interesting exercise in topology that $\tau^2 = 1$ and thus the group is $\pi_1(\mathbb{S}^{d-1} / \sim) \cong \mathbb{Z}_2$. Hence, if we assign a complex phase $e^{i\theta}$ to the generator τ representing a simple 2-particle exchange, then in the case $d \geq 3$ we must for consistency have that $e^{i2\theta} = 1$ and hence either $\theta = 0$ or $\theta = \pi$.

Now, very briefly, in the general N -particle case the possibilities for the free kinetic energy operator depend in a similar way critically on the dimension d of the one-particle space, and in particular on the fundamental group π_1 of the N -particle configuration space (again the non-trivial continuous particle exchanges are described by the group of loops in the configuration space modulo homotopy equivalences). This is

$$\pi_1(\mathcal{C}_{\text{sym}}^{d \times N}) = \begin{cases} S_N, & d \geq 3, \\ B_N, & d = 2, \\ 1, & d = 1, \end{cases}$$

where B_N is called the **braid group** on N strands, and 1 is the trivial group. The possible quantizations \hat{T} such that they reduce locally to the usual one for free distinguishable particles are then labeled by (irreducible, unitary) representations of these groups as complex

⁽¹⁶⁾A **loop** γ in a space X is a continuous function $[0, 1] \rightarrow X$ such that its endpoints are identified.

phases, i.e. homomorphisms

$$\rho: \pi_1(\mathcal{C}_{\text{sym}}^{d \times N}) \rightarrow \text{U}(1), \quad (3.50)$$

which in the case $d \geq 3$ of the permutation group reduces to only two possibilities:

$$\rho = 1 \text{ (the trivial representation),} \quad \text{or} \quad \rho = \text{sign}. \quad (3.51)$$

These can be shown to correspond to the bosons respectively fermions defined above, namely, after choosing one of these representations one may in fact consistently extend the configuration space with a patch for each element $\sigma \in S_N$ to obtain $\mathbb{R}^{dN} \setminus \Delta$ with the corresponding N -body wave functions satisfying either (3.47) or (3.48), and after closing up the space $\overline{\mathbb{R}^{dN} \setminus \Delta} = \mathbb{R}^{dN}$ (unambiguous limits) one is finally left with \mathcal{H}_{sym} or $\mathcal{H}_{\text{asym}}$.

On the other hand, in the case $d = 2$ it turns out one has a full unit circle of possibilities:

$$\rho(\tau_j) = e^{i\alpha\pi}, \quad \alpha \in [0, 2) \text{ (periodic)}, \quad (3.52)$$

with α the same for all the generators τ_j , $j = 1, 2, \dots, N - 1$, of the group B_N (see Exercise 3.13). The corresponding particles are called **anyons** (as in ‘any phase’ [Wil82]) with **statistics parameter** α , and in the case $\alpha = 0$ one again has bosons in the above common sense and for $\alpha = 1$ fermions. We shall denote by \hat{T}_α the free kinetic energy operator for anyons, and it turns out that there are two equivalent ways to model them rigorously: either by means of topological boundary conditions, known in the literature as the **anyon gauge picture** (see [MS95, DFT97] and Remark 3.29 below for a proper definition), or using the ordinary bosons $\Psi \in L^2_{\text{sym}}(\mathbb{R}^{2N})$ or fermions $\Psi \in L^2_{\text{asym}}(\mathbb{R}^{2N})$ but with a peculiar (again topological) magnetic interaction, which is known as the **magnetic gauge picture**. Taking bosons at $\alpha = 0$ as reference, the kinetic energy operator in the latter picture is explicitly

$$\hat{T}_\alpha := \sum_{j=1}^N \left(-i\nabla_{\mathbf{x}_j} + \alpha \sum_{k \neq j} \frac{(\mathbf{x}_j - \mathbf{x}_k)^\perp}{|\mathbf{x}_j - \mathbf{x}_k|^2} \right)^2, \quad (3.53)$$

acting on the bosonic Hilbert space $\mathcal{H}_{\text{sym}} = L^2_{\text{sym}}(\mathbb{R}^{2N})$, where $\mathbf{x}^\perp = (x, y)^\perp := (-y, x)$. Note that for $\alpha \neq 0$ this operator is singular at Δ . One may take its Friedrichs extension on the minimal domain $C_c^\infty(\mathbb{R}^{2N} \setminus \Delta) \cap \mathcal{H}_{\text{sym}}$ to define *free* anyons (see [LS14, Section 2.2], [LL18, Section 1.1] and [CO18] for a mathematical discussion of the possible definitions). Indeed there is a periodicity in the parameter α as in (3.52), manifested by conjugating with even powers of the (unitary but also singular at Δ) **Bose-Fermi transmutation**

$$U: \mathcal{H}_{\text{sym}} \rightarrow \mathcal{H}_{\text{asym}}, \quad \mathcal{H}_{\text{asym}} \rightarrow \mathcal{H}_{\text{sym}}, \quad U\Psi(\mathbf{x}) = \prod_{j < k} \exp[i \arg(\mathbf{x}_j - \mathbf{x}_k)] \Psi(\mathbf{x}). \quad (3.54)$$

Finally, in the one-dimensional case it looks as if there are no non-trivial choices since the fundamental group is trivial (the space $\mathcal{C}_{\text{sym}}^{1 \times N}$ is simply connected, geometrically having the form of a wedge-shaped subset of \mathbb{R}^N), however in this case there are other ambiguities leading to different quantizations \hat{T} (see e.g. [Pol99, Myr99] for physical reviews, and [LS14, Section 2.1] for mathematical details). Intuitively, this is because a continuous exchange of two particles on the real line \mathbb{R} necessarily leads to a collision and therefore one needs to prescribe what happens at the collision points, while more formally it is because the removal of the diagonals Δ introduces boundaries in the configuration space and thus demands the specification of boundary conditions. However, most if not all of the known

quantizations can in fact be modeled using bosons or fermions together with some choice of pair interactions W , and thus we will in one dimension only consider the usual bosons (3.47) or fermions (3.48).

Remark 3.27. The observable incorporation (3.45) of the indistinguishability of particles, and its lifting to the phase ambiguity (3.46), or in general (3.50), may be viewed as a consequence of the definition of quantum states in axiom A1, namely that a state is only defined up to an equivalent ray in the Hilbert space \mathcal{H} , and that states that cannot be distinguished by any observable should be identified. Taking into account the overall normalization of the state $\Psi \in \mathcal{H}$, the position observable $\mathbf{x} \in \mathcal{C}_{\text{sym}}^{d \times N}$, and its projection operator $P_{\Omega}^{\mathbf{x}}$, which together determine the amplitude of Ψ at every point, the only remaining ambiguity is the pointwise phase of Ψ (see below for further details).

Also note that, because of the symmetry (3.45), the one-body density (3.41) simplifies to

$$\varrho_{\Psi}(\mathbf{x}) = N \int_{\mathbb{R}^{d(N-1)}} |\Psi(\mathbf{x}, \mathbf{x}_1, \dots, \mathbf{x}_{N-1})|^2 d\mathbf{x}_1 \dots d\mathbf{x}_{N-1}$$

for indistinguishable particles.

Remark 3.28. A further complication, which we will not find room to discuss in detail here, is the concept of **spin**. Namely, *relativistic* quantum mechanics predicts that there must be additional geometric degrees of freedom associated to every particle in the form of a representation of angular momentum, labelled by its spin quantum number (cf. Exercise 3.7), and furthermore that there is a direct connection between spin and statistics; see e.g. [Frö90] for review. We will return to some consequences of this theory in Section 5.2.

*Remark** 3.29. The proper geometric setting to think about the above quantization problem for identical particles is in the language of **fiber bundles** and **connections** (see e.g. [Nak03]). Namely, locally $\Psi: \Omega \subseteq \mathbb{R}^{dN} \rightarrow \mathbb{C}$ is a function, but globally Ψ is a section of a complex line bundle over the configuration space $\mathcal{C}_{\text{sym}}^{d \times N}$. If assumed to be **locally flat** (which physically means that if the particles are not moving too much then they are certainly distinguishable and should thus have the usual free kinetic energy \hat{T}) such bundles/connections are fully classified by the maps (3.50). Furthermore, just as we may have reason to consider a larger Hilbert space $\mathcal{H} = L^2(\mathbb{R}^{dN}; \mathbb{C}^n)$ for distinguishable particles, where \mathbb{C}^n is called an **internal space**, containing additional degrees of freedom on top of the spatial ones, the one-dimensional fiber \mathbb{C} may also be changed to \mathbb{C}^n (or possibly even some infinite-dimensional Hilbert space). For $d = 2$ this leads then to the notion of **non-abelian anyons**, which are classified by irreducible unitary representations

$$\rho: B_N \rightarrow U(n) \tag{3.55}$$

(the ones considered in (3.50) with $n = 1$ are in fact **abelian anyons** since phases commute; a similar generalization also exists in the case $d \geq 3$ but one may then argue that it can be incorporated into the frameworks of ordinary bosons and fermions [Frö90, DR90]).

Let us consider how the above notions arise starting strictly from the axioms of quantum mechanics. We thus attempt to sketch the formal procedure here, although we are not aware of it having been done in complete detail elsewhere (see however [MD93, DGH99, DŠT01]). Assume generally that we have been given a configuration space manifold \mathcal{C} which contains the observable positions $\mathbf{x} \in \mathcal{C}$ of the system and whose topology describes how such positions are logically related. Consider the Borel subsets $\Omega \subseteq \mathcal{C}$, and the corresponding

observables “ $x \in \Omega$ ” $\in \mathcal{O}$. These should be represented by self-adjoint operators “ $\widehat{x \in \Omega}$ ” $\in \mathcal{L}(\mathcal{H})$ on some Hilbert space \mathcal{H} , and must have eigenvalues 0 (false) or 1 (true) to represent the outcome of such a measurement. In other words, these “ $\widehat{x \in \Omega}$ ” $= P_{\Omega}^{\hat{x}} \in \mathcal{B}(\mathcal{H})$ are in fact projection operators on \mathcal{H} . Considering the ranges of such projection operators,

$$\mathfrak{h}_{\Omega} := P_{\Omega}^{\hat{x}}\mathcal{H} \subseteq \mathcal{H},$$

we thus have a correspondence

$$\begin{array}{ccc} \mathfrak{h}_{\Omega} & \subseteq & \mathcal{H} \\ \updownarrow & & \\ P_{\Omega}^{\hat{x}} & \in & \mathcal{B}(\mathcal{H}) \\ \updownarrow & & \\ \Omega & \subseteq & \mathcal{C} \end{array}$$

between Borel subsets of \mathcal{C} and closed subspaces of \mathcal{H} .

Now take a smaller subset $\Omega' \subseteq \Omega$ and observe that clearly

$$“x \in \Omega'” \Rightarrow “x \in \Omega”$$

so that the information brought by the former observable is finer than that brought by the latter, implying $P_{\Omega'}^{\hat{x}} P_{\Omega}^{\hat{x}} = P_{\Omega'}^{\hat{x}}$, and therefore $\mathfrak{h}_{\Omega'} \hookrightarrow \mathfrak{h}_{\Omega}$. Also, one may consider two subsets $\Omega_i, \Omega_j \subseteq \mathcal{C}$, and in the case that they overlap $\Omega_i \cap \Omega_j \neq \emptyset$ we have two diagrams

$$\begin{array}{ccc} \Omega_i & \Omega_j & \\ \cup & \cup & \\ \Omega_i \cap \Omega_j & & \end{array} \quad \text{and} \quad \begin{array}{ccc} \mathfrak{h}_{\Omega_i} & \mathfrak{h}_{\Omega_j} & \\ \uparrow & \uparrow & \\ \mathfrak{h}_{\Omega_i \cap \Omega_j} & & \end{array}. \quad (3.56)$$

Thus, one may relate the space \mathfrak{h}_{Ω_i} to \mathfrak{h}_{Ω_j} , and vice versa, via the intersecting space $\mathfrak{h}_{\Omega_i \cap \Omega_j}$.

Consider now the particular system at hand, that is the configuration space $\mathcal{C} = \mathcal{C}_{\text{sym}}^{d \times N}$ of N indistinguishable particles on \mathbb{R}^d . We start from the classical expression for the kinetic energy

$$T(\mathbf{p}) = \frac{1}{2m} \sum_{j=1}^N |\mathbf{p}_j|^2 \in \mathcal{O},$$

where $\mathbf{p} \in T_{\mathbf{x}}^*(\mathcal{C}) \cong \mathbb{R}^{dN}$ is the cotangent vector at $\mathbf{x} \in \mathcal{C}$, and wish to look for quantizations \hat{T} represented on a corresponding Hilbert space \mathcal{H} . We require that any such quantization must reduce to the usual one (3.35) for distinguishable particles as soon as the particles indeed are distinguishable. In other words, upon restricting to a small enough subset $\Omega \subseteq \mathcal{C}$ — thereby imposing the knowledge with certainty that the particles are distinguishable — we may consider the corresponding subspace $\mathfrak{h}_{\Omega} = P_{\Omega}^{\hat{x}}\mathcal{H}$ as sitting in some Hilbert space $\mathcal{H}_{\text{dist}}$ of distinguishable particles. By the Stone–von Neumann uniqueness theorem (see Remark 3.13), with $\mathbf{x} \in \mathbb{R}^{dN}$ and $\mathbf{p} \in \mathbb{R}^{dN}$ satisfying the CCR (3.3)/(3.18) and represented as self-adjoint operators on $\mathcal{H}_{\text{dist}}$, we must have $\mathcal{H}_{\text{dist}} \cong L^2(\mathbb{R}^{dN}) \otimes \mathcal{F}$ for some Hilbert space \mathcal{F} on which any remaining observables $a \in \mathcal{O}$ of the system may be represented (we are here relaxing the irreducibility requirement in the Schrödinger representation in order to be as general as possible and allow for other observables).

More precisely, and in order to also take operator domain issues into account, we may initially consider states $\Psi \in \mathcal{H}$ that are completely localized on topologically trivial subsets $\mathcal{C} \supseteq \Omega_j \hookrightarrow \mathbb{R}^{dN} \setminus \Delta$ of configurations of distinguishable particles. We thus take such $\Psi \in \mathfrak{h}_{\Omega_j}$

and furthermore demand that $0 \leq \langle T(\hat{p}) \rangle_\Psi < \infty$ in order for such states to be physical. The Hilbert space on which we represent \hat{x} as a multiplication operator and $\hat{p} = -i\hbar\nabla$ as a differentiation operator, in order to implement the CCR and the Weyl algebra, is then $L^2(\Omega_j; \mathcal{F}_j) \cong L^2(\Omega_j) \otimes \mathcal{F}_j \subseteq \mathcal{H}_{\text{dist}}$ for some undetermined space $\mathcal{F}_j \subseteq \mathcal{F}$. Taking the minimal domain, $\Psi \in C_c^\infty(\Omega_j; \mathcal{F}_j)$, certainly ensures that states are physical with finite kinetic energy and amounts, upon taking the closure of such states, to a form domain $\mathcal{Q}(\hat{T}) = H_0^1(\Omega_j; \mathcal{F}_j)$, i.e. the Dirichlet realization of \hat{T} on Ω_j . On the other hand, one may also consider a *maximal* domain, namely any states $\Psi \in L^2(\Omega_j; \mathcal{F}_j)$ for which one can make finite sense of the form $\langle \Psi, \hat{T}\Psi \rangle = (2m)^{-1} \|\nabla\Psi\|^2$, which is $\mathcal{Q}(\hat{T}) = \mathcal{D}(\nabla) = H^1(\Omega_j; \mathcal{F}_j)$, the Neumann realization for distinguishable particles on Ω_j . Since the former domain sits in the latter, and we should try to be as unrestrictive as possible in our choices, let us then only require that $\mathfrak{h}_{\Omega_j} \cong L^2(\Omega_j; \mathcal{F}_j) \ni \Psi$ with $(\hat{x}\Psi)(\mathbf{x}) = \mathbf{x}\Psi(\mathbf{x})$ and $(\hat{p}\Psi)(\mathbf{x}) = -i\hbar\nabla\Psi(\mathbf{x})$ s.t. $\int_{\Omega_j} \|\nabla\Psi\|_{\mathcal{F}}^2 < \infty$ for any physical states Ψ .

Hence we have obtained for each topologically trivial $\Omega_j \subseteq \mathcal{C}$ an isomorphism $\mathfrak{h}_{\Omega_j} \cong L^2(\Omega_j) \otimes \mathcal{F}_j$. Let us then cover \mathcal{C} by a finite collection $\{\Omega_j\}_{j \in J}$ of suitable such subsets. In the case of $N = 2$ we may for example choose as Ω_j , in terms of relative coordinates (\mathbf{X}, \mathbf{r}) ,

$$\Omega_j = \left\{ [(\mathbf{x}_1, \mathbf{x}_2)] \in \mathcal{C}_{\text{sym}}^{d \times 2} : \mathbf{X} \in \mathbb{R}^d, \mathbf{r} = r\omega, r > 0, \omega \in B_\varepsilon(\mathbf{n}_j) \cap \mathbb{S}^{d-1} \right\}$$

where $\{\mathbf{n}_j\} \subseteq \mathbb{S}^{d-1}$ is a finite collection of unit vectors and $\varepsilon > 0$ is small enough. Furthermore, we may impose the symmetry in the system on the collection $\{\Omega_j\}_{j \in J}$ by requiring that the subsets are related $\Omega_i = R_{ij}\Omega_j$ via symmetry transformations $R_{ij}: \mathbb{R}^{dN} \rightarrow \mathbb{R}^{dN}$ which extend to unitary operators $U_{ij}: \mathfrak{h}_{\Omega_j} \rightarrow \mathfrak{h}_{\Omega_i}$. We must therefore for all $i, j \in J$ have that

$$L^2(\Omega_i) \otimes \mathcal{F}_i \cong \mathfrak{h}_{\Omega_i} \cong \mathfrak{h}_{\Omega_j} \cong L^2(\Omega_j) \otimes \mathcal{F}_j$$

and hence, since $L^2(\Omega_i) \cong L^2(\Omega_j)$, we find that $\mathcal{F}_i \cong \mathcal{F}_j \forall i, j \in J$. Let us therefore denote this prototype **fiber Hilbert space** by \mathcal{F} .

Coming back to the general observation (3.56), now with $\mathfrak{h}_{\Omega_j} \cong L^2(\Omega_j) \otimes \mathcal{F}$ for each subset of the covering $\{\Omega_j\}$, we must on the subspace

$$L^2(\Omega_i; \mathcal{F}) \supseteq L^2(\Omega_i \cap \Omega_j; \mathcal{F}) \hookrightarrow \mathfrak{h}_{\Omega_i \cap \Omega_j} \hookrightarrow L^2(\Omega_i \cap \Omega_j; \mathcal{F}) \subseteq L^2(\Omega_j; \mathcal{F})$$

have an isomorphism acting locally in the fiber \mathcal{F} ,

$$t_{ij}: L^2(\Omega_i \cap \Omega_j; \mathcal{F}) \subseteq L^2(\Omega_i; \mathcal{F}) \rightarrow L^2(\Omega_j; \mathcal{F}), \quad t_{ij}(\mathbf{x}) \in \text{U}(\mathcal{F}).$$

The data $(\{\Omega_j\}, \{t_{ij}\}, \mathcal{F})$ defines a vector bundle $E \rightarrow \mathcal{C}$ with structure group $G = \text{U}(\mathcal{F})$ whose geometry is encoded in the transition functions $\{t_{ij}\}$ and the connection. Given that the connection is flat on each local piece Ω_j (the operator $i\hat{p}$ is the usual gradient ∇ on a piece of flat \mathbb{R}^{dN}) and that transitions ought to be trivial whenever particles remain distinguishable, we thus have a locally flat bundle, whose only non-trivial geometry is classified using the non-trivial topology of \mathcal{C} , more precisely the fundamental group $\pi_1(\mathcal{C})$ (a well-known correspondence; see e.g. [MD93] and [Mic13, Chapter 5] for details), by homomorphisms (representations)

$$\rho: \pi_1(\mathcal{C}) \rightarrow \text{U}(\mathcal{F}).$$

In the case that $\mathcal{F} \cong \mathbb{C}$ resp. $\mathcal{F} \cong \mathbb{C}^n$ this then reduces to (3.50) resp. (3.55). In general the dimension n of the fiber \mathcal{F} would depend on whether there are additional observables in \mathcal{O}

which could distinguish n . If there are no such observables, then we should, by demanding that all states be distinguishable (irreducibility), simply take $n = 1$.

We considered above local sections $\Psi \in L^2(\Omega_j; \mathcal{F}) \subseteq \Gamma(\Omega_j, E)$ which should be extended to *continuous* global sections on E , for example by taking the closure of smooth sections. The full Hilbert space is then the space of square-integrable sections

$$\mathcal{H} = \left\{ \Psi \in \Gamma(\mathcal{C}; E) : \int_{\mathcal{C}} \|\Psi\|_{\mathcal{F}}^2 < \infty \right\},$$

with the local requirement $\int_{\Omega_j} \|\nabla\Psi\|_{\mathcal{F}}^2 < \infty$ for physical states $\Psi \in \Gamma(\Omega_j, E)$ then lifting globally to yield the form domain

$$\mathcal{Q}(\hat{T}) = \left\{ \Psi \in \mathcal{H} : \int_{\mathcal{C}} \|\nabla\Psi\|_{\mathcal{F}}^2 < \infty \right\}.$$

By its non-negativity, this form $q_{\hat{T}}: \mathcal{Q}(\hat{T}) \rightarrow \mathbb{R}_+$ finally defines for us a *unique* (given the bundle E , i.e. the representation ρ) non-negative self-adjoint operator $\hat{T} = \hat{T}_{\rho} \in \mathcal{L}(\mathcal{H})$, which reduces on each local domain Ω_j to the usual free kinetic energy (3.35) for distinguishable particles with domains $\mathcal{Q}(\hat{T}|_{\Omega_j}) = H^1(\Omega_j; \mathcal{F})$ and $\mathcal{D}(\hat{T}|_{\Omega_j}) \subseteq H^2(\Omega_j; \mathcal{F})$.

In the case $d = 2$ and $\mathcal{F} \cong \mathbb{C}$ with (3.52) one may further trivialize the transition functions $t_{ij} \in \text{U}(1)$ on the bundle by the (singular) gauge transformation [Wu84a, Wu84b, Dow85]

$$\Psi \mapsto U^{\alpha}\Psi,$$

where $U = U(x)$ in (3.54), resulting in the magnetic gauge picture for abelian anyons defined by the operator $\hat{T}_{\alpha} = U^{-\alpha}\hat{T}_{\rho}U^{\alpha}$ in (3.53).

Note that the procedure of defining \hat{T} by means of the form domain really does matter, namely if we start for simplicity from the flat but punctured bundle of distinguishable particles $E = (\mathbb{R}^{dN} \setminus \Delta) \times \mathcal{F}$ with trivial transition functions and consider all possible operator extensions from the minimal domain $C_c^{\infty}(\mathbb{R}^{dN} \setminus \Delta; \mathcal{F})$, then those may (if $d \leq 3$) include **point interactions** [AGHKH05, BS92]. However, by considering instead the form domain as above one obtains for $d \geq 2$ *uniquely* the extension corresponding to free particles, with $\mathcal{Q}(\hat{T}) = H^1(\mathbb{R}^{dN}; \mathcal{F})$ and $\mathcal{D}(\hat{T}) = H^2(\mathbb{R}^{dN}; \mathcal{F})$ (see [LS14] for the critical case $d = 2$).

We should finally remark that the choice of observables employed above corresponds to the usual Schrödinger representation over an exchange-symmetric geometry. However, one could alternatively start from a different choice of exchange-symmetric observables, such as

$$A = x^2, \quad B = p^2, \quad C = \frac{1}{2}(xp + px),$$

where $x \in \mathbb{R}$ is a relative coordinate and p its momentum, and actually arrive at a *different* family of quantizations. This approach has been referred to in the literature as the **Heisenberg representation** for identical particles (see e.g. [Myr99]).

Exercise 3.13. *The braid group B_N can be defined as the abstract group generated by elements τ_j , $j = 1, 2, \dots, N - 1$, (and their inverses) satisfying the **braid relations***

$$\tau_j\tau_k = \tau_k\tau_j, \quad \text{for } |j - k| \geq 2, \quad \text{and} \quad \tau_j\tau_{j+1}\tau_j = \tau_{j+1}\tau_j\tau_{j+1}, \quad 1 \leq j \leq N - 2,$$

(the latter are also called **Yang-Baxter relations**). *Show that these relations imply that if $\rho: B_N \rightarrow \text{U}(1)$ is a representation, i.e. a homomorphism $\rho(xy) = \rho(x)\rho(y)$, then it is uniquely defined by its values on the generators $\rho(\tau_j) = e^{i\alpha_j\pi}$, $j = 1, 2, \dots, N - 1$, and*

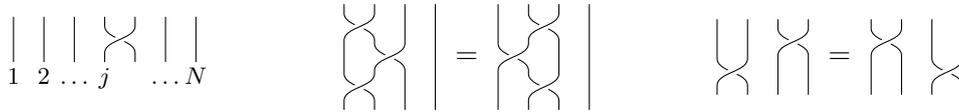


FIGURE 1. Braid diagrams corresponding to the generator τ_j of B_N , i.e. a counterclockwise exchange of particles/strands j and $j+1$ with time running upwards, and the relations $\tau_1\tau_2\tau_1 = \tau_2\tau_1\tau_2$ respectively $\tau_1\tau_3 = \tau_3\tau_1$ of B_4 .

furthermore that $e^{i\alpha_1\pi} = \dots = e^{i\alpha_{N-1}\pi} =: e^{i\alpha\pi}$. Also, show that if the additional relations $\tau_j^2 = 1, j = 1, \dots, N - 1$, are added then the resulting group is S_N and that the only possibilities for ρ are then (3.51).

Exercise 3.14. We may represent a general particle exchange in two dimensions, or an element of B_N , using a **braid diagram**, i.e. an arbitrary composition of **simple braids** of N strands, with each simple braid τ_j formed by taking the j :th strand over the $j+1$:st strand; see Figure 3.7. Show using such braid diagrams that if the phase associated to a simple two-particle exchange is $\rho(\tau_j) = e^{i\alpha\pi}$, then the phase that will arise as one particle encircles p other particles in a simple loop is $e^{i2p\alpha\pi}$, while if a pair of particles is exchanged once and in the exchange loop they enclose p other particles then the phase must be $e^{i(2p+1)\alpha\pi}$.

Exercise 3.15. Consider the corresponding braid group defined with the particles situated on the surface of the sphere S^2 instead of \mathbb{R}^2 . Show that in this case there is an extra topological condition on the generators,

$$\tau_1\tau_2 \dots \tau_{N-1}\tau_{N-1} \dots \tau_2\tau_1 = 1,$$

and determine the possible values of the statistics parameter α .

4. UNCERTAINTY PRINCIPLES

We will now investigate the most important feature of quantum mechanics as compared to classical mechanics, namely the consequence of the non-commutativity of position and momentum observables referred to as the **uncertainty principle**. Namely, as made famous by Heisenberg, for two non-commuting observables a and b and a state $\psi \in \mathcal{H}$, we have that

$$\left\langle (\hat{a} - \langle \hat{a} \rangle_\psi)^2 \right\rangle_\psi \left\langle (\hat{b} - \langle \hat{b} \rangle_\psi)^2 \right\rangle_\psi \geq \frac{1}{4} \left| \langle [\hat{a}, \hat{b}] \rangle_\psi \right|^2 = \frac{\hbar^2}{4} \left| \langle \widehat{\{a, b\}} \rangle_\psi \right|^2.$$

On the l.h.s. stands the product of the variances of a measurement of a and b , while the r.h.s. depends on the quantization of the observable $\{a, b\}$ and its expectation in ψ , which in the case that $\{a, b\} = \text{const.} \neq 0$ is strictly positive independently of ψ . Therefore this inequality has the physical interpretation that it is *impossible* to know the value of both a and b simultaneously to arbitrary precision. The most important case is the canonical position and momentum operators, \hat{x}_j and \hat{p}_k , and we will in this section formulate various versions of the uncertainty principle involving these operators. We set $\hbar = 1$ for simplicity.

Exercise 4.1. *Prove the more general relation, known as the **Robertson–Schrödinger uncertainty relation**, (with ψ in a common dense domain of all the operators)*

$$\left\langle (\hat{a} - \langle \hat{a} \rangle_\psi)^2 \right\rangle_\psi \left\langle (\hat{b} - \langle \hat{b} \rangle_\psi)^2 \right\rangle_\psi \geq \left| \frac{1}{2} \langle \hat{a}\hat{b} + \hat{b}\hat{a} \rangle_\psi - \langle \hat{a} \rangle_\psi \langle \hat{b} \rangle_\psi \right|^2 + \left| \frac{1}{2} \langle [\hat{a}, \hat{b}] \rangle_\psi \right|^2,$$

by considering $\langle f, g \rangle$ with $f = (\hat{a} - \langle \hat{a} \rangle_\psi)\psi$ and $g = (\hat{b} - \langle \hat{b} \rangle_\psi)\psi$.

4.1. Heisenberg. Recall the canonical commutation relations (3.18),

$$[\hat{x}_j, \hat{p}_k] = i\delta_{jk}\mathbb{1}.$$

In particular,

$$i(\hat{\mathbf{p}} \cdot \hat{\mathbf{x}} - \hat{\mathbf{x}} \cdot \hat{\mathbf{p}}) = i \sum_{j=1}^d (\hat{p}_j \hat{x}_j - \hat{x}_j \hat{p}_j) = \sum_{j=1}^d \delta_{jj} \mathbb{1} = d\mathbb{1},$$

or in the usual Schrödinger representation (∇ here acts as an operator on everything to the right)

$$\nabla \cdot \mathbf{x} - \mathbf{x} \cdot \nabla = d\mathbb{1}. \quad (4.1)$$

This identity can be used together with the Cauchy-Schwarz inequality to prove the most famous version of the uncertainty principle of quantum mechanics:

Theorem 4.1 (Heisenberg’s uncertainty principle). *For any $\psi \in L^2(\mathbb{R}^d)$ with $\|\psi\|_{L^2} = 1$, we have*

$$\langle \psi, \hat{\mathbf{p}}^2 \psi \rangle \langle \psi, \hat{\mathbf{x}}^2 \psi \rangle \geq \frac{d^2}{4}. \quad (4.2)$$

Remark 4.2. By means of the Fourier transform, the l.h.s. should be understood to be

$$\int_{\mathbb{R}^d} |\nabla \psi(\mathbf{x})|^2 d\mathbf{x} \int_{\mathbb{R}^d} |\mathbf{x}\psi(\mathbf{x})|^2 d\mathbf{x} = \int_{\mathbb{R}^d} |\mathbf{p}\hat{\psi}(\mathbf{p})|^2 d\mathbf{p} \int_{\mathbb{R}^d} |\mathbf{x}\psi(\mathbf{x})|^2 d\mathbf{x},$$

which is finite if and only if both these integrals converge, i.e. $\psi \in H^1(\mathbb{R}^d) \cap \mathcal{D}(\hat{\mathbf{x}})$. Moreover, by replacing $\psi(\mathbf{x})$ by $e^{i\mathbf{x} \cdot \mathbf{p}_0} \psi(\mathbf{x} + \mathbf{x}_0)$, the inequality may also be written

$$\langle (\hat{\mathbf{p}} - \mathbf{p}_0)^2 \rangle_\psi \langle (\hat{\mathbf{x}} - \mathbf{x}_0)^2 \rangle_\psi \geq \frac{d^2}{4}. \quad (4.3)$$

This formulation of the uncertainty principle is the original and most well-known one [Hei27], and indeed it tells us that if the state ψ localizes around the origin so that the r.h.s. of the inequality

$$\langle \psi, \hat{\mathbf{p}}^2 \psi \rangle \geq \frac{d^2}{4} \langle \psi, \hat{\mathbf{x}}^2 \psi \rangle^{-1} \quad (4.4)$$

tends to infinity, then this also implies a large momentum. However, as stressed e.g. in [Lie76] (see also [LS10]), this is unfortunately not sufficient for proving stability of the hydrogenic atom. Namely, the expectation value $\langle \psi, \hat{\mathbf{x}}^2 \psi \rangle$ is a poor measure of how localized the state is, since it is possible to make this value very large without changing the kinetic energy much. Consider for example the state

$$\psi(\mathbf{x}) = \sqrt{1 - \varepsilon^2} u(\mathbf{x}) + \varepsilon v(\mathbf{x} - \mathbf{y}),$$

with $\varepsilon \in (0, 1)$, $u, v \in C_c^\infty(B_1(0))$ normalized in L^2 , and $|\mathbf{y}| > 2$. Then $\int_{\mathbb{R}^d} |\psi|^2 = 1$ and

$$\int_{\mathbb{R}^d} |\mathbf{x}|^2 |\psi(\mathbf{x})|^2 d\mathbf{x} = (1 - \varepsilon^2) \int_{B_1(0)} |\mathbf{x}|^2 |u(\mathbf{x})|^2 d\mathbf{x} + \varepsilon^2 \int_{B_1(0)} |\mathbf{y} + \mathbf{z}|^2 |v(\mathbf{z})|^2 d\mathbf{z} \geq \varepsilon^2 (|\mathbf{y}| - 1)^2,$$

while

$$\int_{\mathbb{R}^d} |\nabla \psi(\mathbf{x})|^2 d\mathbf{x} = (1 - \varepsilon^2) \int_{B_1(0)} |\nabla u(\mathbf{x})|^2 d\mathbf{x} + \varepsilon^2 \int_{B_1(0)} |\nabla v(\mathbf{x})|^2 d\mathbf{x}.$$

Hence, we may take simultaneously $\varepsilon \ll 1$ and $|\mathbf{y}| \gg \varepsilon^{-1}$ to make the r.h.s. of (4.4) small while the l.h.s. stays essentially the same.

Before considering formulations that are more useful for our stability problem, we note that there is also the following version of the Heisenberg uncertainty principle which explains that a state $\psi \in \mathcal{H} \setminus \{0\}$ and its Fourier transform $\hat{\psi}$ cannot both have compact support (see e.g. [Tes14, Theorem 7.12] for a proof, and e.g. [Ben85, Hed12] for various generalizations):

Theorem 4.3. *Suppose $f \in L^2(\mathbb{R}^n)$. If both f and \hat{f} have compact support, then $f = 0$.*

In other words, recalling our interpretations of $|\psi(\mathbf{x})|^2$ respectively $|\hat{\psi}(\mathbf{p})|^2$ for a normalized state ψ as probability densities for the observables \mathbf{x} respectively \mathbf{p} , this theorem tells us that it is impossible to know with certainty that both $\mathbf{x} \in B_R(0)$ and $\mathbf{p} \in B_{R'}(0)$, regardless of the size of the radii $R, R' > 0$. Furthermore, in any possible state of the system at least one of these conjugate observables must take arbitrarily large values.

Exercise 4.2. *Prove (4.2) and (4.3) for $\psi \in C_c^\infty(\mathbb{R}^d)$ by taking expectation values of the relation (4.1). How can this be extended to $L^2(\mathbb{R}^d)$?*

Exercise 4.3. *Check that the **Gaussian wave packet***

$$\psi(x) = (\lambda/\pi)^{1/4} e^{-\frac{\lambda}{2}|x-x_0|^2 + ip_0 x},$$

for any $\lambda > 0$, is normalized and realizes the minimum of (4.3) in dimension $d = 1$.

4.2. Hardy. A more powerful version of the uncertainty principle is Hardy's inequality:

Theorem 4.4 (The Hardy inequality). *For any $u \in H^1(\mathbb{R}^d)$ in dimension $d \geq 2$, and for any $u \in H_0^1(\mathbb{R} \setminus \{0\})$ in dimension $d = 1$, we have that*

$$\int_{\mathbb{R}^d} |\nabla u(\mathbf{x})|^2 d\mathbf{x} \geq \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|u(\mathbf{x})|^2}{|\mathbf{x}|^2} d\mathbf{x}. \quad (4.5)$$

Remark 4.5. The constant $(d-2)^2/4$ is sharp (and the inequality trivial for $d=2$), in the sense that for any larger constant there is a function $u \in C_c^\infty(\mathbb{R}^d \setminus \{0\})$ which violates it (see below and e.g. [Lun15, Appendix B] for a continued discussion).

Remark 4.6. The inequality (4.5) of quadratic forms translates to the following operator inequality:

$$-\Delta \geq \frac{(d-2)^2}{4} \frac{1}{|\mathbf{x}|^2},$$

with both sides interpreted as non-negative operators on $L^2(\mathbb{R}^d)$ having a common form domain $\mathcal{Q}(-\Delta_{\mathbb{R}^d}) = H^1(\mathbb{R}^d)$, $d \geq 2$, respectively $\mathcal{Q}(-\Delta_{\mathbb{R} \setminus \{0\}}) = H_0^1(\mathbb{R} \setminus \{0\})$.

Many other types of Hardy inequalities exist, and their general defining characteristic is that they provide a bound for the Laplacian (and hence for the kinetic energy \hat{T}) from below in terms of a positive potential V which scales in the same way, i.e. as an inverse-square length or distance, and which is singular at some point of the configuration space or its boundary. In other words, in case such a non-trivial inequality holds, we clearly have that the kinetic energy is not only non-negative but it even tends to infinity if the state is sufficiently localized close to such a singularity of V . We refer to the recent book [BEL15] and the more classic references given in [Tid05] for general treatments of Hardy inequalities. Although the basic inequality (4.5) is fairly straightforward to prove directly, we will instead take a very general approach to proving Hardy inequalities, involving a formulation referred to as the ‘ground state representation’. This approach is not covered by the above standard references but has been discussed in various forms in for example [Bir61, AHKS77, FS08, FSW08, Sei10, Lun15].

Exercise 4.4. Show that $\langle \psi, |\mathbf{x}|^{-2} \psi \rangle \geq \langle \psi, |\mathbf{x}|^2 \psi \rangle^{-1}$ if $\|\psi\| = 1$, and hence that Hardy (4.5) directly implies Heisenberg (4.2) but with a slightly weaker constant.

4.2.1. *The ground state representation.* We consider the following identity involving the quadratic form of the Dirichlet Laplacian on a domain in \mathbb{R}^n , which we refer to as the **ground state representation (GSR)**:

Proposition 4.7 (GSR). Let Ω be an open set in \mathbb{R}^n and let $f: \Omega \rightarrow \mathbb{R}^+ := (0, \infty)$ be twice differentiable. Then, for any $u \in C_c^\infty(\Omega)$ and $\alpha \in \mathbb{R}$,

$$\int_{\Omega} |\nabla u|^2 = \int_{\Omega} \left(\alpha(1-\alpha) \frac{|\nabla f|^2}{f^2} + \alpha \frac{-\Delta f}{f} \right) |u|^2 + \int_{\Omega} |\nabla v|^2 f^{2\alpha}, \quad (4.6)$$

where $v = f^{-\alpha} u$.

Proof. We have for $u = f^\alpha v$ that $\nabla u = \alpha f^{\alpha-1} (\nabla f) v + f^\alpha \nabla v$, and hence

$$|\nabla u|^2 = \alpha^2 f^{2(\alpha-1)} |\nabla f|^2 |v|^2 + \alpha f^{2\alpha-1} (\nabla f) \cdot \nabla |v|^2 + f^{2\alpha} |\nabla v|^2.$$

Now let us integrate this expression over Ω , and note that the middle term on the r.h.s. produces after a partial integration (note that v vanishes on $\partial\Omega$)

$$-\alpha \int_{\Omega} |v|^2 \nabla \cdot (f^{2\alpha-1} \nabla f).$$

Finally, using that

$$\nabla \cdot (f^{2\alpha-1} \nabla f) = (2\alpha-1) f^{2\alpha-2} |\nabla f|^2 + f^{2\alpha-1} \Delta f,$$

and collecting the terms we arrive at (4.6). \square

The idea of the ground state representation is to factor out a positive function f^α from the kinetic energy form, to the cost of a new potential

$$\alpha(1 - \alpha) \frac{|\nabla f|^2}{f^2} + \alpha \frac{-\Delta f}{f}, \quad (4.7)$$

which we will call the **GSR potential**. Note that if f is chosen to be an exact zero-eigenfunction of the Laplacian, $\Delta f = 0$, i.e. a harmonic function, or a **generalized ground state** of the kinetic energy operator (not necessarily normalizable on $L^2(\Omega)$ or in the form domain), then the last term of (4.7) vanishes while the first is positive and maximal for the choice $\alpha = 1/2$. Since the last integral in (4.6) is also non-negative this then yields a potentially useful estimate of the kinetic energy form in terms of this positive potential. Also in the case that f is not an exact zero-eigenfunction but for example an approximation to the true ground state, the first term in the potential (4.7) may still be able to control the second one and produce a useful positive bound. The parameter α may then be used in a variational sense to find the best possible bound given the ansatz f , which if the exact ground state is unknown instead may be taken of a form which is convenient for computations.

Exercise 4.5. Show that a modification of Proposition 4.7 to involve a product ground state ansatz $g^\alpha h^\beta$ (i.e. $u = g^\alpha h^\beta v$) produces the corresponding GSR potential

$$\alpha(1 - \alpha) \frac{|\nabla g|^2}{g^2} + \alpha \frac{-\Delta g}{g} + \beta(1 - \beta) \frac{|\nabla h|^2}{h^2} + \beta \frac{-\Delta h}{h} - 2\alpha\beta \frac{\nabla g \cdot \nabla h}{gh}. \quad (4.8)$$

Exercise 4.6. Apply the ground state approach to prove a Hardy inequality on $[0, 1]$, i.e. find functions g and h on $[0, 1]$ s.t. $g(0) = 0$ and $g'' = 0$, and $h(1) = 0$ and $h'' = 0$, compute the GSR potential (4.8) and try to optimize it w.r.t. α and β .

4.2.2. *The standard Hardy inequalities in \mathbb{R}^d .* Our approach to prove the standard Hardy inequality (4.5) is to first prove that it holds for all $u \in C_c^\infty(\mathbb{R}^d \setminus \{0\})$ (this is a minimal domain respecting the singularity of the potential) using the above ground state representation, and then conclude that it also holds on the Sobolev space $H_0^1(\mathbb{R}^d \setminus \{0\})$ by density. Finally, we prove that actually $H_0^1(\mathbb{R}^d \setminus \{0\}) = H^1(\mathbb{R}^d)$ if the dimension d is large enough, a result which is also very useful in itself.

A natural choice of ground states f for the Laplacian in \mathbb{R}^d are the **fundamental solutions**:

$$\begin{aligned} d \neq 2 : & & f_d(\mathbf{x}) &:= |\mathbf{x}|^{-(d-2)}, & \Delta_{\mathbb{R}^d} f_d &= c_d \delta_0, \\ d = 2 : & & f_2(\mathbf{x}) &:= \ln |\mathbf{x}|, & \Delta_{\mathbb{R}^2} f_2 &= c_2 \delta_0, \end{aligned} \quad (4.9)$$

where δ_0 are Dirac delta distributions supported at the origin and c_d some constants which only depend on d (see Exercise 4.7). These functions are smooth and strictly positive for all $\mathbf{x} \neq \mathbf{0}$ if $d \neq 2$, while for $d = 2$ we may cure the sign problem by taking absolute values, but still need to avoid both the origin $\mathbf{x} = \mathbf{0}$ and the circle $|\mathbf{x}| = 1$ (a different nonzero radius may be chosen by rescaling). Indeed we cannot expect to have a non-trivial Hardy inequality on all of \mathbb{R}^2 , as indicated by the vanishing constant in (4.5).

Hence, for $d \neq 2$ we consider the domain $\Omega := \mathbb{R}^d \setminus \{0\}$, on which $f := f_d > 0$ and $\Delta f = 0$, while $|\nabla f|^2/f^2 = (d-2)^2/|\mathbf{x}|^2$. The GSR potential (4.7) is therefore optimal for

$\alpha = \frac{1}{2}$, and (4.6) yields the ground state representation associated to the standard Hardy inequality (4.5) in \mathbb{R}^d :

$$\int_{\Omega} |\nabla u(\mathbf{x})|^2 d\mathbf{x} - \frac{(d-2)^2}{4} \int_{\Omega} \frac{|u(\mathbf{x})|^2}{|\mathbf{x}|^2} d\mathbf{x} = \int_{\Omega} |\nabla v(\mathbf{x})|^2 |\mathbf{x}|^{-(d-2)} d\mathbf{x} \geq 0. \quad (4.10)$$

The inequality (4.10) thus holds for all $u \in C_c^\infty(\Omega)$. Now, if we take an arbitrary function u in the Sobolev space $H_0^1(\Omega)$, then we have by its definition a sequence $(u_n) \subset C_c^\infty(\Omega)$ s.t.

$$\int_{\Omega} |u - u_n|^2 \rightarrow 0, \quad \text{and} \quad \int_{\Omega} |\nabla(u - u_n)|^2 \rightarrow 0.$$

We then find by (4.10) that this sequence is also Cauchy in the space $L^2(\Omega, |\mathbf{x}|^{-2} d\mathbf{x})$ weighted by the singular GSR potential:

$$\int_{\Omega} |u_n - u_m|^2 |\mathbf{x}|^{-2} d\mathbf{x} \leq \frac{4}{(d-2)^2} \int_{\Omega} |\nabla(u_n - u_m)|^2 \rightarrow 0,$$

which implies for the limit $u \in L^2(\Omega, |\mathbf{x}|^{-2} d\mathbf{x})$. Furthermore, taking $n \rightarrow \infty$,

$$\int_{\Omega} |u - u_m|^2 |\mathbf{x}|^{-2} d\mathbf{x} \leq \frac{4}{(d-2)^2} \int_{\Omega} |\nabla(u - u_m)|^2 \rightarrow 0,$$

and therefore, by approximating both sides of the desired inequality in terms of $u_m \in C_c^\infty$,

$$\int_{\Omega} |u|^2 |\mathbf{x}|^{-2} d\mathbf{x} \leq \frac{4}{(d-2)^2} \int_{\Omega} |\nabla u|^2,$$

which proves the Hardy inequality (4.5) on the space $H_0^1(\mathbb{R}^d \setminus \{0\}) \subseteq H^1(\mathbb{R}^d)$.

It remains then to prove that actually $H_0^1(\mathbb{R}^d \setminus \{0\}) = H^1(\mathbb{R}^d)$, so that the Hardy inequality indeed holds on the maximal form domain of the Laplacian.

Lemma 4.8. *We have that $H_0^1(\mathbb{R}^d \setminus \{0\}) = H^1(\mathbb{R}^d)$ for $d \geq 2$.*

Remark 4.9. It is not true that $H_0^1(\mathbb{R} \setminus \{0\}) = H^1(\mathbb{R})$, but one rather has a decomposition

$$H_0^1(\mathbb{R} \setminus \{0\}) \cong H_0^1(\mathbb{R}_-) \oplus H_0^1(\mathbb{R}_+)$$

in one dimension.

Proof of Lemma 4.8. We aim to prove that $C_c^\infty(\mathbb{R}^d \setminus \{0\})$ is dense in $H^1(\mathbb{R}^d)$. Since $C_c^\infty(\mathbb{R}^d)$ is dense in $H^1(\mathbb{R}^d)$ (recall from Section 2.4 that we have $H_0^1(\mathbb{R}^d) = H^1(\mathbb{R}^d)$) it suffices to prove that an arbitrary $u \in C_c^\infty(\mathbb{R}^d)$ can be approximated arbitrarily well by a sequence $(u_n) \subset C_c^\infty(\mathbb{R}^d \setminus \{0\})$ in the $H^1(\mathbb{R}^d)$ -norm. For $d \geq 3$ we take a cut-off function $\varphi \in C^\infty(\mathbb{R}^d; [0, 1])$ such that $\varphi(\mathbf{x}) = 0$ for $|\mathbf{x}| \leq 1$ and $\varphi(\mathbf{x}) = 1$ for $|\mathbf{x}| \geq 2$, and let

$$u_\varepsilon(\mathbf{x}) := \varphi_\varepsilon(\mathbf{x})u(\mathbf{x}), \quad \varphi_\varepsilon(\mathbf{x}) := \varphi(\mathbf{x}/\varepsilon),$$

for $\varepsilon > 0$. Then $u_\varepsilon \in C_c^\infty(\mathbb{R}^d \setminus B_\varepsilon(0))$ and, as $\varepsilon \rightarrow 0$,

$$\|u - u_\varepsilon\|_{L^2}^2 = \int_{\mathbb{R}^d} |u - u_\varepsilon|^2 = \int_{\mathbb{R}^d} |u|^2 |1 - \varphi_\varepsilon|^2 \leq \int_{B_{2\varepsilon}(0) \setminus B_\varepsilon(0)} C \rightarrow 0.$$

Furthermore, by the product rule and the triangle inequality,

$$\|\nabla(u - u_\varepsilon)\|_{L^2} \leq \|(1 - \varphi_\varepsilon)\nabla u\|_{L^2} + \|(\nabla\varphi_\varepsilon)u\|_{L^2},$$

with $\|(1 - \varphi_\varepsilon)\nabla u\|_{L^2}^2 \rightarrow 0$ as above and

$$\|(\nabla\varphi_\varepsilon)u\|_{L^2}^2 = \int_{\mathbb{R}^d} |u|^2 |\nabla\varphi_\varepsilon|^2 \leq C \int_{B_{2\varepsilon}(0) \setminus B_\varepsilon(0)} |\nabla\varphi_\varepsilon|^2 \leq C\varepsilon^{-2} |B_{2\varepsilon}(0)| \leq C\varepsilon^{d-2} \rightarrow 0,$$

as $\varepsilon \rightarrow 0$.

In the case $d = 2$ the above choice fails but we may instead take $\varphi_\varepsilon(\mathbf{x}) = \varphi(\varepsilon \ln |\mathbf{x}|)$ with $\varphi \in C^\infty(\mathbb{R}; [0, 1])$ such that $\varphi = 0$ on $(-\infty, -2)$ and $\varphi = 1$ on $(-1, \infty)$. Then $u_\varepsilon := \varphi_\varepsilon u \in C_c^\infty(\mathbb{R}^2 \setminus B_{e^{-2/\varepsilon}}(0))$, and again $\|u - u_\varepsilon\|_{L^2} \rightarrow 0$ and $\|(1 - \varphi_\varepsilon)\nabla u\|_{L^2} \rightarrow 0$ as above. Moreover, by first switching to polar coordinates and then making the change of variable $r = e^s$,

$$\frac{1}{2\pi} \int_{\mathbb{R}^2} |\nabla\varphi_\varepsilon|^2 d\mathbf{x} = \varepsilon^2 \int_0^\infty |\varphi'(\varepsilon \ln r)|^2 \frac{dr}{r} = \varepsilon^2 \int_{-2/\varepsilon}^{-1/\varepsilon} |\varphi'(\varepsilon s)|^2 ds \leq C\varepsilon \rightarrow 0,$$

as $\varepsilon \rightarrow 0$, which completes the proof. \square

The above proves Theorem 4.4, and may also be straightforwardly generalized in numerous directions. For $d = 2$ we can instead take the two-component domain $\Omega := \mathbb{R}^2 \setminus (\{0\} \cup \mathbb{S}^1)$ and the ground state $f := |f_2|$, so that $f > 0$ and $\Delta f = 0$ on Ω . Also, $|\nabla f(\mathbf{x})| = 1/|\mathbf{x}|$. Proposition 4.7 then produces the corresponding two-dimensional GSR for $u \in C_c^\infty(\Omega)$

$$\int_\Omega |\nabla u|^2 d\mathbf{x} - \frac{1}{4} \int_\Omega \frac{|u(\mathbf{x})|^2}{|\mathbf{x}|^2 (\ln |\mathbf{x}|)^2} d\mathbf{x} = \int_\Omega |\nabla v|^2 |\ln |\mathbf{x}|| d\mathbf{x} \geq 0. \quad (4.11)$$

By taking the closure of $u \in C_c^\infty(\Omega)$ as above and using Lemma 4.8 locally around the point $\mathbf{0}$, the l.h.s. of (4.11) is non-negative for all $u \in H_0^1(\Omega) = H_0^1(\mathbb{R}^2 \setminus \mathbb{S}^1)$. Hence we proved the following two-dimensional Hardy inequality:

Theorem 4.10. *For any $u \in H_0^1(\mathbb{R}^2 \setminus \mathbb{S}^1)$ we have that*

$$\int_{\mathbb{R}^2} |\nabla u|^2 d\mathbf{x} \geq \frac{1}{4} \int_{\mathbb{R}^2} \frac{|u(\mathbf{x})|^2}{|\mathbf{x}|^2 (\ln |\mathbf{x}|)^2} d\mathbf{x}. \quad (4.12)$$

Also note that we are free to choose the location of the singularity in the Hardy inequality, namely by translation invariance of the kinetic energy we also have for example

$$\int_{\mathbb{R}^d} |\nabla u(\mathbf{x})|^2 d\mathbf{x} \geq \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|u(\mathbf{x})|^2}{|\mathbf{x} - \mathbf{x}_0|^2} d\mathbf{x},$$

for any $\mathbf{x}_0 \in \mathbb{R}^d$ and $u \in H^1(\mathbb{R}^d)$, $d \geq 3$, respectively $u \in H_0^1(\mathbb{R}^1 \setminus \{\mathbf{x}_0\})$.

Exercise 4.7. *Verify that (4.9) are the fundamental solutions, i.e. zero-eigenfunctions of the Laplacian outside $\mathbf{0}$, and, if you know distribution theory, compute the constants c_d (i.e. consider $\int_{\mathbb{R}^d} f \Delta \varphi$ for $\varphi \in C_c^\infty(\mathbb{R}^d)$ and make partial integrations).*

Exercise 4.8. *Prove that the inequality (4.12) does not extend to $H^1(\mathbb{R}^2)$.*

Exercise 4.9. *Prove a Hardy inequality outside the hard-sphere potential of Example 3.20 in $d = 3$, by taking the ground state $f(\mathbf{x}) = 1 - R/|\mathbf{x}|$. Can it be improved by using an additional ground state $g(\mathbf{x}) = 1/|\mathbf{x}|$?*

4.2.3. *Many-body Hardy inequalities.* In [Tid05, HOHOLT08] a number of interesting and useful many-body versions of the Hardy inequality were derived. Some of these were extended geometrically in [Lun15]. We only mention the simplest, one-dimensional, case here, and return to some other, fermionic as well as anyonic, versions in conjunction with exclusion principles in Section 5.

Recall the definition (3.49) of the many-body configuration space diagonal Δ .

Theorem 4.11. *For any $u \in H_0^1(\mathbb{R}^N \setminus \Delta)$ we have that*

$$\int_{\mathbb{R}^N} |\nabla u|^2 dx \geq \frac{1}{2} \sum_{1 \leq j < k \leq N} \int_{\mathbb{R}^N} \frac{|u(x)|^2}{|x_j - x_k|^2} dx.$$

This inequality is useful for the analysis of **Calogero–Sutherland** [Cal71, Sut71] and similar models in many-body quantum mechanics involving inverse-square interactions. It proves immediately that an interacting many-body Hamiltonian of the form

$$\hat{H}^N = \hat{T} + \beta \hat{W} = - \sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + \beta \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|^2},$$

with form domain $\mathcal{Q}(\hat{H}^N) = H_0^1(\mathbb{R}^N \setminus \Delta)$, is trivially **stable** (of both first and second kind) if the interaction coupling strength parameter satisfies $\beta \geq -1/2$, i.e. if it is not too attractive.

Exercise 4.10. *Prove that for any three distinct points $x_1, x_2, x_3 \in \mathbb{R}$,*

$$(x_1 - x_2)^{-1}(x_1 - x_3)^{-1} + (x_2 - x_3)^{-1}(x_2 - x_1)^{-1} + (x_3 - x_1)^{-1}(x_3 - x_2)^{-1} = 0.$$

Exercise 4.11. *Use this identity and the ansatz $f(x) := \prod_{j < k} |x_j - x_k|$ on $\Omega := \mathbb{R}^N \setminus \Delta$ to prove the one-dimensional many-body GSR*

$$\int_{\Omega} |\nabla u|^2 dx - \frac{1}{2} \sum_{j < k} \int_{\Omega} \frac{|u(x)|^2}{|x_j - x_k|^2} dx = \int_{\Omega} |\nabla(f^{-1/2}u)|^2 f \geq 0,$$

for $u \in C_c^\infty(\Omega)$, and hence Theorem 4.11.

4.3. **Sobolev.** Another very powerful formulation of the uncertainty principle is given by Sobolev's inequality:

Theorem 4.12 (The Sobolev inequality). *For $d \geq 3$ and all $u \in H^1(\mathbb{R}^d)$, it holds that*

$$\int_{\mathbb{R}^d} |\nabla u|^2 \geq S_d \|u\|_{2d/(d-2)}^2, \quad (4.13)$$

with $S_d = d(d-2)|\mathbb{S}^d|^{2/d}/4$. For $d = 2$ and every $2 < p < \infty$ there exists a constant $S_{2,p} > 0$ such that for any $u \in H^1(\mathbb{R}^2)$,

$$\int_{\mathbb{R}^2} |\nabla u|^2 \geq S_{2,p} \|u\|_2^{-4/(p-2)} \|u\|_p^{2p/(p-2)}. \quad (4.14)$$

For $d = 1$ one has for $u \in H^1(\mathbb{R})$,

$$\int_{\mathbb{R}} |u'|^2 \geq \|u\|_2^{-2} \|u\|_\infty^4. \quad (4.15)$$

Remark 4.13. In (4.13) the assumption $u \in H^1(\mathbb{R}^d)$ may be weakened slightly but vanishing at infinity is of course required; see [LL01, Section 8.2-8.3].

The constants S_d respectively $S_1 = 1$ in the case $d \geq 3$ and $d = 1$ are sharp (see [Aub75, Tal76], and e.g. [LL01]), with $S_3 = 3(\pi/2)^{4/3} \approx 5.478$, while the value of the optimal constant $S_{2,p}$ for $d = 2$ is presently unknown (a very rough but explicit estimate may be obtained from [LL01, Theorem 8.5]). Also note as usual the necessary match of dimensions in these inequalities (cf. the remark after Proposition 2.7) which not only helps to remember them but also clarifies why an inequality of the simpler form (4.13) cannot extend to $d \leq 2$.

Proof for $d = 1$. By the fundamental theorem of calculus applied to an approximating sequence $u_n \in C_c^\infty(\mathbb{R})$ (see [LL01, Theorem 8.5] for details), one has for any $u \in H^1(\mathbb{R})$ and a.e. $x \in \mathbb{R}$

$$u(x)^2 = \int_{-\infty}^x u(y)u'(y) dy - \int_x^{\infty} u(y)u'(y) dy.$$

Therefore, by the triangle inequality,

$$|u(x)|^2 \leq \int_{-\infty}^x |u||u'| + \int_x^{\infty} |u||u'| = \int_{-\infty}^{\infty} |u||u'|,$$

and thus by the Cauchy–Schwarz inequality,

$$\|u\|_\infty^2 \leq \|u\|_2 \|u'\|_2,$$

which is (4.15). □

We shall not give a proof of Theorem 4.12 for $d = 2$ for general $p > 2$ here, but refer instead to e.g. [LL01, Theorem 8.5]. A proof for the important special case $p = 4$ will be given below. For $d \geq 3$ we follow a proof which is closer in spirit to those of upcoming specializations of the uncertainty principle, and which was given in [Len13] based on [CX97]. It also generalizes straightforwardly to fractional Sobolev spaces but does not yield the optimal constant S_d however.

Proof for $d \geq 3$. Let $u \in H^1(\mathbb{R}^d)$ and set $q = 2d/(d-2)$. Using the unitary Fourier transform $\hat{u} = \mathcal{F}u$ we may decompose u into low- and high-frequency parts, $u = u_P^- + u_P^+$, with

$$u_P^- := \mathcal{F}^{-1} [\mathbf{1}_{B_P(0)} \hat{u}] \quad \text{and} \quad u_P^+ := \mathcal{F}^{-1} [\mathbf{1}_{B_P(0)^c} \hat{u}],$$

for an arbitrary momentum/frequency $P > 0$ to be chosen below. We then use that

$$\|u\|_q^q = \int_{t=0}^{\infty} |\{|u| > t\}| d(t^q), \tag{4.16}$$

by the layer-cake representation (2.5), and that by the triangle inequality $|u| \leq |u_P^-| + |u_P^+|$,

$$\{|u| > t\} \subseteq \{|u_P^-| > t/2\} \cup \{|u_P^+| > t/2\}. \tag{4.17}$$

Now, note that by the Fourier inversion formula, $\|f\|_\infty \leq (2\pi)^{-d/2} \|\hat{f}\|_1$, so that

$$\begin{aligned} (2\pi)^{d/2} \|u_P^-\|_\infty &\leq \|\mathcal{F}u_P^-\|_1 = \int_{B_P(0)} \frac{1}{|\mathbf{p}|} |\mathbf{p}\hat{u}(\mathbf{p})| d\mathbf{p} \leq \left(\int_{B_P(0)} \frac{d\mathbf{p}}{|\mathbf{p}|^2} \right)^{1/2} \|\mathcal{F}(\nabla u)\|_2 \\ &= \left(\frac{|\mathbb{S}^{d-1}|}{d-2} \right)^{1/2} P^{\frac{d-2}{2}} \|\nabla u\|_2, \end{aligned}$$

by Cauchy–Schwarz. Hence, if we choose

$$P = P(t) := \left(\frac{(d-2)(2\pi)^d t^2}{|\mathbb{S}^{d-1}| \|\nabla u\|_2^2 4} \right)^{\frac{1}{d-2}} =: C_d(t/\|\nabla u\|_2)^{\frac{2}{d-2}}$$

then $|\{|u_P^-| > t/2\}| = 0$, and we obtain in (4.16)-(4.17)

$$\|u\|_q^q \leq \int_{t=0}^\infty |\{|u_{P(t)}^+| > t/2\}| d(t^q) \leq \int_{t=0}^\infty 4\|u_{P(t)}^+\|_2^2/t^2 d(t^q),$$

by Chebyshev's inequality (2.6). Thus,

$$\|u\|_q^q \leq 4q \int_0^\infty \|\mathcal{F}u_{P(t)}^+\|_2^2 t^{q-3} dt = 4q \int_0^\infty \int_{B_{P(t)}(0)^c} |\hat{u}(\mathbf{p})|^2 d\mathbf{p} t^{q-3} dt,$$

and by Fubini's theorem and inverting the relation

$$|\mathbf{p}| \geq P(t) \Leftrightarrow t \leq \|\nabla u\|_2 (|\mathbf{p}|/C_d)^{\frac{d-2}{2}} =: \Lambda(\mathbf{p}),$$

we have

$$\begin{aligned} \|u\|_q^q &\leq 4q \int_{\mathbb{R}^d} |\hat{u}(\mathbf{p})|^2 \int_0^{\Lambda(\mathbf{p})} t^{q-3} dt d\mathbf{p} = \frac{4q}{q-2} C_d^{-2} \|\nabla u\|^{q-2} \int_{\mathbb{R}^d} |\hat{u}(\mathbf{p})|^2 |\mathbf{p}|^2 d\mathbf{p} \\ &= 2dC_d^{-2} \|\nabla u\|^q. \end{aligned}$$

This proves the Sobolev inequality (4.13) with the constant

$$S'_d = (2dC_d^{-2})^{-2/q} = \frac{(2\pi)^2}{(2d)^{\frac{d-2}{d}}} \left(\frac{d-2}{4} \right)^{\frac{2}{d}} |\mathbb{S}^{d-1}|^{-\frac{2}{d}},$$

which for $d = 3$ is $S'_3 = \pi^{4/3}/(2 \cdot 3^{1/3}) \approx 1.595$. \square

4.3.1. Sobolev from Hardy. Alternatively, the Sobolev inequality for $d \geq 3$ actually also follows from the Hardy inequality, by the method of rearrangements; see [FS08, Sei10]. Namely, for any radial, non-negative decreasing function $u: \mathbb{R}^d \rightarrow \mathbb{R}_+$ one has the inequality

$$\|u\|_p^p = \int_{\mathbb{R}^d} u(\mathbf{y})^p d\mathbf{y} \geq u(\mathbf{x})^p |\mathbf{x}|^d |\mathbb{B}^d|$$

for any $\mathbf{x} \in \mathbb{R}^d$ and $p > 2$, where $\mathbb{B}^d = B_1(0)$ denotes the unit ball in \mathbb{R}^d . Taking both sides to the power $1 - 2/p$, multiplying by $u(\mathbf{x})^2 |\mathbf{x}|^{-d(1-2/p)}$ and integrating over \mathbf{x} , one obtains

$$\int_{\mathbb{R}^d} \frac{u(\mathbf{x})^2}{|\mathbf{x}|^{d(1-2/p)}} d\mathbf{x} \geq |\mathbb{B}^d|^{1-2/p} \|u\|_p^2.$$

Taking $p = 2d/(d-2)$, the l.h.s. reduces to the r.h.s. of the Hardy inequality (4.5) and thus Hardy implies Sobolev for such $u \in H^1(\mathbb{R}^d)$. Finally, one may use a symmetric-decreasing

rearrangement (we refer to e.g. [LL01, Chapter 3] for details) to reduce an arbitrary $u \in H^1(\mathbb{R}^d)$ to such a non-negative decreasing radial function u^* , with the properties $\|u\|_p = \|u^*\|_p$ and $\|\nabla u\|_2 \geq \|\nabla u^*\|_2$. The first property follows by the layer-cake representation while last property is the non-trivial one, and it would be too much of a detour to try to cover this approach here.

4.4. Gagliardo–Nirenberg–Sobolev. Note that by an application of Hölder’s inequality, for $d \geq 3$,

$$\int_{\mathbb{R}^d} |u|^{2(1+2/d)} \leq \|u\|_2^{4/d} \|u\|_{2d/(d-2)}^2, \quad (4.18)$$

and thus by the Sobolev inequality (4.13),

$$\left(\int_{\mathbb{R}^d} |\nabla u|^2 \right) \left(\int_{\mathbb{R}^d} |u|^2 \right)^{2/d} \geq S_d \int_{\mathbb{R}^d} |u|^{2(1+2/d)}. \quad (4.19)$$

This is another formulation of the uncertainty principle known as a **Gagliardo–Nirenberg–Sobolev (GNS) inequality**. Note that such an inequality also follows in $d = 2$ directly from (4.14) with $p = 4$, and that in $d = 1$ one has from (4.15) that

$$\int_{\mathbb{R}} |u|^6 \leq \|u\|_\infty^4 \|u\|_2^2 \leq \|u\|_2^4 \|u'\|_2^2.$$

Hence (4.19) takes the same form in all dimensions $d \geq 1$, and we shall here present an independent and simple proof for it which also allows for many useful generalizations (this is the one-body version of a proof due to Rumin of a more general kinetic energy inequality, which will be given later in Theorem 6.1).

Theorem 4.14 (Gagliardo–Nirenberg–Sobolev inequality — one-body version). *For any $d \geq 1$ there exists a constant $G_d > 0$ such that for all $u \in H^1(\mathbb{R}^d)$*

$$\int_{\mathbb{R}^d} |\nabla u|^2 \geq G_d \left(\int_{\mathbb{R}^d} |u|^2 \right)^{-2/d} \int_{\mathbb{R}^d} |u|^{2(1+2/d)}. \quad (4.20)$$

Remark 4.15. The optimal constant satisfies $G_1 = \pi^2/4 > 1$, $G_2 = S_{2,4}$, respectively $G_d \geq S_d$ for $d \geq 3$, and for all $d \geq 1$ we also have the explicit lower bound

$$G_d \geq G'_d := \frac{(2\pi)^2 d^{2+2/d} |\mathbb{S}^{d-1}|^{-2/d}}{(d+2)(d+4)}. \quad (4.21)$$

The exact value of the optimal constant $G_{d \geq 2}$ is presently unknown but numerical work suggests $G_3 \approx 9.578$, to be contrasted with $S_3 \approx 5.478$ and $G'_3 \approx 3.907$ (see [LT76, Lie76], and also [Lev14] for more recent related numerical work, as well as [BVV18b, FHJN18]).

Proof. We decompose an arbitrary $u \in H^1(\mathbb{R}^d)$ into parts corresponding to low respectively high kinetic energy according to $u = u_{E,-} + u_{E,+}$, with an energy cut-off $E > 0$, and

$$u_{E,-} := \mathcal{F}^{-1} [\mathbf{1}_{\{|\mathbf{p}|^2 \leq E\}} \hat{u}] \quad \text{and} \quad u_{E,+} := \mathcal{F}^{-1} [\mathbf{1}_{\{|\mathbf{p}|^2 > E\}} \hat{u}].$$

Then by the unitarity of the Fourier transform, and Fubini,

$$\begin{aligned} \int_0^\infty \int_{\mathbb{R}^d} |u_{E,+}(\mathbf{x})|^2 d\mathbf{x} dE &= \int_0^\infty \int_{\mathbb{R}^d} |\widehat{u_{E,+}}(\mathbf{p})|^2 d\mathbf{p} dE = \int_{\mathbb{R}^d} \int_0^{|\mathbf{p}|^2} |\hat{u}(\mathbf{p})|^2 dE d\mathbf{p} \\ &= \int_{\mathbb{R}^d} |\mathbf{p}|^2 |\hat{u}(\mathbf{p})|^2 d\mathbf{p} = \int_{\mathbb{R}^d} |\nabla u(\mathbf{x})|^2 d\mathbf{x}. \end{aligned} \quad (4.22)$$

For the low-energy part we use that by Fourier inversion and Cauchy–Schwarz

$$\begin{aligned} |u_{E,-}(\mathbf{x})| &= \left| (2\pi)^{-d/2} \int_{\mathbb{R}^d} \mathbf{1}_{\{|\mathbf{p}|^2 \leq E\}} \hat{u}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} d\mathbf{p} \right| \\ &\leq (2\pi)^{-d/2} |B_{E^{1/2}}(0)|^{1/2} \|\hat{u}\|_2 = (2\pi)^{-d/2} d^{-1/2} |\mathbb{S}^{d-1}|^{1/2} E^{d/4} \|u\|_2. \end{aligned} \quad (4.23)$$

Now, combining (4.22) and (4.23) with the pointwise triangle inequality

$$|u_{E,+}(\mathbf{x})| \geq \left[|u(\mathbf{x})| - |u_{E,-}(\mathbf{x})| \right]_+, \quad (4.24)$$

yields the bound

$$\int_{\mathbb{R}^d} |\nabla u(\mathbf{x})|^2 d\mathbf{x} \geq \int_0^\infty \int_{\mathbb{R}^d} \left[|u(\mathbf{x})| - (2\pi)^{-d/2} d^{-1/2} |\mathbb{S}^{d-1}|^{1/2} \|u\|_2 E^{d/4} \right]_+^2 d\mathbf{x} dE.$$

Again changing the order of integration and then carrying out the integral over E , with

$$\int_0^\infty \left[A - Bt^{d/4} \right]_+^2 dt = \frac{d^2 A^{2+4/d} B^{-4/d}}{(d+2)(d+4)}, \quad (4.25)$$

one finally obtains

$$\int_{\mathbb{R}^d} |\nabla u(\mathbf{x})|^2 d\mathbf{x} \geq \frac{(2\pi)^2 d^{2+2/d} |\mathbb{S}^{d-1}|^{-2/d}}{(d+2)(d+4)} \|u\|_2^{-4/d} \int_{\mathbb{R}^d} |u|^{2(1+2/d)}.$$

This also produces the bound (4.21) for the optimal constant G_d while for $d \geq 3$ this may be improved by (4.19). \square

We have also the following many-body version of the GNS inequality:

Theorem 4.16 (Gagliardo–Nirenberg–Sobolev inequality — many-body version). *For any $d \geq 1$, $N \geq 1$, and every L^2 -normalized N -body state $\Psi \in H^1(\mathbb{R}^{dN})$,*

$$\sum_{j=1}^N \int_{\mathbb{R}^{dN}} |\nabla_j \Psi|^2 \geq G_d N^{-2/d} \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d},$$

where the constant G_d is the same as in Theorem 4.14.

This can be proved either by directly generalizing the above proof (Exercise 4.13) or by using the following inequality and then an application of Theorem 4.14 to $u = \sqrt{\varrho_\Psi}$.

Lemma 4.17 (Hoffmann–Ostenhof inequality). *For any $d \geq 1$, $N \geq 1$, and every L^2 -normalized N -body state $\Psi \in H^1(\mathbb{R}^{dN})$,*

$$\sum_{j=1}^N \int_{\mathbb{R}^{dN}} |\nabla_j \Psi|^2 \geq \int_{\mathbb{R}^d} |\nabla \sqrt{\varrho_\Psi}|^2. \quad (4.26)$$

The inequality (4.26) is actually equivalent to its one-body version, i.e. the simple inequality

$$\int_{\mathbb{R}^d} |\nabla u|^2 \geq \int_{\mathbb{R}^d} |\nabla |u||^2. \quad (4.27)$$

This is known as a **diamagnetic inequality** because it holds in greater generality also involving magnetic fields, namely the gradient $\nabla u \approx e^{i(\arg u)} \nabla |u| + iu \nabla(\arg u)$ may be replaced by $(\nabla + i\mathbf{A})u$, where $\mathbf{A} \in L^2_{\text{loc}}(\mathbb{R}^d; \mathbb{R}^d)$ is a magnetic vector potential (see e.g. [LL01, Theorem 7.21] for a proof). The many-body version (4.26) was first proved in [HH77] (see also e.g. [Lew15, Lemma 3.2] for a simple generalization and proof).

Exercise 4.12. *Prove the inequality (4.18).*

Exercise 4.13. *Prove Theorem 4.16 by defining for each $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{x}_{j+1}, \dots, \mathbf{x}_N) \in \mathbb{R}^{d(N-1)}$ a collection of functions*

$$u_j(\mathbf{x}, \mathbf{x}') := \Psi(\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{x}, \mathbf{x}_{j+1}, \dots, \mathbf{x}_N)$$

and using instead of (4.24) the triangle inequality on $L^2(\mathbb{R}^{d(N-1)}; \mathbb{C}^N)$,

$$\begin{aligned} & \left(\int_{\mathbb{R}^{d(N-1)}} \sum_{j=1}^N |u_j^{E,+}(\mathbf{x}, \mathbf{x}')|^2 d\mathbf{x}' \right)^{1/2} \\ & \geq \left[\left(\int_{\mathbb{R}^{d(N-1)}} \sum_{j=1}^N |u_j(\mathbf{x}, \mathbf{x}')|^2 d\mathbf{x}' \right)^{1/2} - \left(\int_{\mathbb{R}^{d(N-1)}} \sum_{j=1}^N |u_j^{E,-}(\mathbf{x}, \mathbf{x}')|^2 d\mathbf{x}' \right)^{1/2} \right]_+. \end{aligned}$$

4.5. Applications to stability. In this subsection we follow mainly [Lie76, LS10, Sei10].

4.5.1. The stability of the hydrogenic atom. We now return to the hydrogenic atom of Example 3.19, which after factoring out the free center-of-mass kinetic energy leaves the more relevant relative Hamiltonian operator on the space $\mathcal{H} = L^2(\mathcal{C}_{\text{rel}}) = L^2(\mathbb{R}^3)$:

$$\hat{H}_{\text{rel}} = -\Delta - \frac{Z}{|\mathbf{x}|}. \quad (4.28)$$

Here we have put for simplicity $2\mu = 1$ for the reduced mass or, equivalently, rescaled the operator and the value of Z , which is no loss in generality. This operator should be understood to be defined via the energy form

$$\mathcal{E}[\psi] := q_{\hat{H}_{\text{rel}}}(\psi) = \left\langle \psi, \left[-\Delta - \frac{Z}{|\mathbf{x}|} \right] \psi \right\rangle_{L^2(\mathbb{R}^3)} = \int_{\mathbb{R}^3} |\nabla \psi|^2 - Z \int_{\mathbb{R}^3} \frac{|\psi(\mathbf{x})|^2}{|\mathbf{x}|} d\mathbf{x},$$

where we may take ψ in the minimal form domain $C_c^\infty(\mathbb{R}^3 \setminus \{0\})$ or the larger closed domain $\mathcal{Q}(\hat{H}_{\text{rel}}) = H^1(\mathbb{R}^3)$ if we just require finite kinetic energy. The self-adjoint realization of \hat{H}_{rel} associated to this form (the Friedrichs extension) then has the ground-state energy

$$E_0 = \inf \{ \mathcal{E}[\psi] : \psi \in H^1(\mathbb{R}^3), \|\psi\|_2 = 1 \}.$$

Using Heisenberg's uncertainty principle (4.4), one has the bound

$$\mathcal{E}[\psi] \geq \frac{9}{4} \left(\int_{\mathbb{R}^3} |\mathbf{x}|^2 |\psi(\mathbf{x})|^2 d\mathbf{x} \right)^{-1} - Z \int_{\mathbb{R}^3} \frac{|\psi(\mathbf{x})|^2}{|\mathbf{x}|} d\mathbf{x}, \quad (4.29)$$

whose r.h.s. can be made arbitrarily negative (Exercise 4.14), therefore not being able to settle the stability question. However, using instead the Hardy inequality (4.5), we obtain the lower bound

$$\mathcal{E}[\psi] \geq \int_{\mathbb{R}^3} \left[\frac{1}{4|\mathbf{x}|^2} - \frac{Z}{|\mathbf{x}|} \right] |\psi(\mathbf{x})|^2 d\mathbf{x}. \quad (4.30)$$

We may then proceed by minimizing the expression in brackets pointwise:

$$\min_{\mathbf{x} \in \mathbb{R}^3} \left[\frac{1}{4|\mathbf{x}|^2} - \frac{Z}{|\mathbf{x}|} \right] = -Z^2, \quad \text{for } |\mathbf{x}| = \frac{1}{2Z},$$

and by the normalization of ψ we therefore obtain the finite lower bound

$$E_0 \geq -Z^2, \quad (4.31)$$

and thus stability for the hydrogenic atom for any finite charge $Z > 0$ (and it is trivially stable for $Z \leq 0$ according to our definitions). In summary, we have thus found that the uncertainty principle introduces an effective repulsion around the origin which overcomes the attraction from the nucleus by its stronger scaling property, scaling quadratically in the inverse distance as opposed to linearly, here resulting in an equilibrium around $|\mathbf{x}| = 1/(2Z)$.

Another approach is to use the Gagliardo–Nirenberg–Sobolev inequality (4.20), that is

$$\mathcal{E}[\psi] \geq G_3 \int_{\mathbb{R}^3} |\psi|^{10/3} - Z \int_{\mathbb{R}^3} \frac{|\psi(\mathbf{x})|^2}{|\mathbf{x}|} d\mathbf{x}, \quad (4.32)$$

with the constant $G_3 \geq S_3 \approx 5.478$. In this case we are led to a constrained optimization problem for the density $\varrho := |\psi|^2$,

$$E_0 \geq \inf \left\{ \int_{\mathbb{R}^3} \left(G_3 \varrho(\mathbf{x})^{5/3} - Z \frac{\varrho(\mathbf{x})}{|\mathbf{x}|} \right) d\mathbf{x} : \varrho: \mathbb{R}^3 \rightarrow \mathbb{R}_+, \int_{\mathbb{R}^3} \varrho = 1 \right\}. \quad (4.33)$$

The minimum can be shown (Exercise 4.16) to be

$$-9(\pi/2)^{4/3} Z^2 / (5G_3) \geq -3Z^2/5 \quad (4.34)$$

for

$$\varrho(\mathbf{x}) = \left(\frac{3}{5} \frac{Z}{G_3} (|\mathbf{x}|^{-1} - R^{-1})_+ \right)^{3/2},$$

with $R = \frac{3}{5}(2/\pi)^{4/3} G_3/Z$. Therefore the GNS inequality, which arose as a weaker implication of the Sobolev inequality (and thus a yet weaker implication of the Hardy inequality), is still strong enough to enforce stability. One may even note that formally replacing the exponent 10/3 in the kinetic term in (4.32) by anything strictly greater than 3, i.e. the 5/3 in (4.33) by any exponent $p > 3/2$ (which would require the constant G_3 to be dimensionful however), would have been sufficient for stability (exercise).

It is actually possible to solve for the complete spectrum $\sigma(\hat{H}_{\text{rel}})$ of the hydrogenic atom, which was indeed worked out shortly after the birth of quantum mechanics. In particular, the exact ground state may be seen to be (with a normalization constant $C > 0$)

$$\psi_0(\mathbf{x}) = C e^{-Z|\mathbf{x}|/2},$$

since this function is positive, square-integrable, and solves the Schrödinger eigenvalue equation

$$\hat{H}_{\text{rel}} \psi_0 = \left(-\Delta - \frac{Z}{|\mathbf{x}|} \right) \psi_0 = -\frac{Z^2}{4} \psi_0 \quad (4.35)$$

(see e.g. [LS10, Section 2.2.2] and [LL01, Section 11.10] for details). Thus, by the min-max principle we have

$$\mathcal{E}[\psi] = \int_{\mathbb{R}^3} |\nabla\psi|^2 - Z \int_{\mathbb{R}^3} \frac{|\psi(\mathbf{x})|^2}{|\mathbf{x}|} d\mathbf{x} \geq -\frac{Z^2}{4} \int_{\mathbb{R}^3} |\psi(\mathbf{x})|^2 d\mathbf{x}$$

for all $\psi \in \mathcal{Q}(\hat{H}_{\text{rel}})$. We thus see that the above-obtained bounds using the Hardy and Sobolev/GNS uncertainty principles are quite close to the actual ground-state energy $E_0 = -Z^2/4$. Moreover, the entire spectrum of the operator (4.28) turns out to be (see e.g. [Tes14, Chapter 10])

$$\sigma(\hat{H}_{\text{rel}}) = \left\{ -\frac{Z^2}{4(n+1)^2} \right\}_{n=0,1,2,\dots} \cup [0, \infty).$$

The infinite sequence of negative eigenvalues of finite multiplicity are the energy levels of the bound electron, with eigenstates corresponding to the ground state and the excited orbitals of the atom, while the non-negative essential spectrum describes states where the electron is not bound to the nucleus but rather scatters off of it, i.e. **scattering states**.

Exercise 4.14. *Prove that the r.h.s. of (4.29) tends to $-\infty$ for some sequence of L^2 -normalized states $\psi \in H^1(\mathbb{R}^d)$.*

Exercise 4.15. *Prove stability of (4.28) from Hardy in a different way than (4.30), using Hölder on the negative term.*

Exercise 4.16. *Compute the minimizer for the variational problem (4.33) in the generalized case with exponent $p > 3/2$ (why is this bound necessary?), and the minimum (4.34) in the case $p = 5/3$.*

Exercise 4.17. *Verify the Schrödinger equation (4.35). How can we be sure that ψ_0 is the ground state?*

4.5.2. *General criteria for stability of the first kind.* In the case of a one-body Schrödinger Hamiltonian operator $\hat{H} = -\Delta + V$ on $\mathcal{H} = L^2(\mathbb{R}^d)$ with a general potential $V: \mathbb{R}^d \rightarrow \mathbb{R}$, $d \geq 3$, we have using Sobolev that for all $\psi \in H^1(\mathbb{R}^d)$

$$\mathcal{E}[\psi] := q_{\hat{H}}(\psi) = \int_{\mathbb{R}^d} |\nabla\psi|^2 + \int_{\mathbb{R}^d} V|\psi|^2 \geq S_d \|\psi\|_{2d/(d-2)}^2 + \int_{\mathbb{R}^d} (V_+ - |V_-|)|\psi|^2,$$

with $V_{\pm} := (V \pm |V|)/2$. Furthermore, if $V_- \in L^{d/2}(\mathbb{R}^d)$ then we have using Hölder that

$$\int_{\mathbb{R}^d} |V_-||\psi|^2 \leq \|V_-\|_{d/2} \|\psi\|_{2d/(d-2)}^2,$$

and therefore

$$\mathcal{E}[\psi] \geq (S_d - \|V_-\|_{d/2}) \|\psi\|_{2d/(d-2)}^2.$$

Assuming $\|V_-\|_{d/2} \leq S_d$ then implies $\mathcal{E}[\psi] \geq 0$, and hence clearly stability for such potentials. However, one may also extract an arbitrary negative constant from the potential without changing this conclusion. In general, if

$$V(\mathbf{x}) = U(\mathbf{x}) + v(\mathbf{x}),$$

where $U \geq -C$, i.e. $U_- \in L^\infty(\mathbb{R}^d)$, and $v \in L^{d/2}(\mathbb{R}^d)$, then by the layer-cake principle there exists for any $\varepsilon \in (0, 1)$ some constant $A_\varepsilon \geq 0$ such that $\|(A_\varepsilon + v)_-\|_{d/2} \leq \varepsilon S_d$, and thus

$$\begin{aligned} \mathcal{E}[\psi] &= T[\psi] + V[\psi] = (1 - \varepsilon)T[\psi] + \varepsilon T[\psi] + \int (U - A_\varepsilon + (A_\varepsilon + v)_-)|\psi|^2 \\ &\geq (1 - \varepsilon)T[\psi] + \varepsilon T[\psi] - \|U_-\|_\infty - A_\varepsilon - \int |(A_\varepsilon + v)_-||\psi|^2 \\ &\geq (1 - \varepsilon)T[\psi] - \|U_-\|_\infty - A_\varepsilon + (\varepsilon S_d - \|(A_\varepsilon + v)_-\|_{d/2})\|\psi\|_{2d/(d-2)}^2 \\ &\geq (1 - \varepsilon)T[\psi] - \|U_-\|_\infty - A_\varepsilon. \end{aligned}$$

This is summarized in the following theorem, where the case $d \leq 2$ is left as an exercise:

Theorem 4.18. *Given a Schrödinger Hamiltonian (3.30) on \mathbb{R}^d with quadratic form*

$$\mathcal{E}[\psi] = \int_{\mathbb{R}^3} (|\nabla\psi|^2 + V|\psi|^2),$$

for some potential $V: \mathbb{R}^d \rightarrow \mathbb{R}$ and finite kinetic energy, $\psi \in H^1(\mathbb{R}^d)$, there is **stability** for the corresponding quantum system, i.e.

$$E_0 = \inf\{\mathcal{E}[\psi] : \psi \in H^1(\mathbb{R}^d), \|\psi\|_2 = 1\} > -\infty,$$

if

$$V_- \in \begin{cases} L^{d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d), & d \geq 3, \\ L^{1+\varepsilon}(\mathbb{R}^2) + L^\infty(\mathbb{R}^2), & d = 2, \\ L^1(\mathbb{R}^1) + L^\infty(\mathbb{R}^1), & d = 1. \end{cases}$$

The Hardy inequality can in fact be even stronger than the above theorem, namely we have immediately by (4.5) that $E_0 > -\infty$ if

$$V(\mathbf{x}) \geq -\frac{(d-2)^2}{4|\mathbf{x}|^2} - C,$$

(note that the r.h.s. is not in $L_{\text{loc}}^{d/2}(\mathbb{R}^d)$ for $d \geq 3$ so Theorem 4.18 does not apply), or even if (exercise)

$$V(\mathbf{x}) \geq -\frac{(d-2)^2}{4} \sum_{k=1}^M |\mathbf{x} - \mathbf{R}_k|^{-2} - C, \quad (4.36)$$

for finitely many distinct points $\mathbf{R}_j \neq \mathbf{R}_k$ in \mathbb{R}^d .

If V_- is not too singular then one may also obtain an explicit bound for E_0 directly from the GNS inequality (4.20), which even turns out to be equivalent to such a bound:

Theorem 4.19 (GNS—Schrödinger equivalence). *The ground-state energy E_0 of the Schrödinger form $\mathcal{E}[\psi]$ in Theorem 4.18 is bounded from below by*

$$E_0 \geq -L_d^1 \int_{\mathbb{R}^d} |V_-|^{1+d/2}, \quad (4.37)$$

with the positive constant $L_d^1 = \frac{2}{d+2} \left(\frac{d}{d+2}\right)^{d/2} G_d^{-d/2}$.

Conversely, if a bound of the form (4.37) holds for arbitrary potentials V and some constant $L_d^1 > 0$, then the GNS inequality (4.20) holds for all $u \in H^1(\mathbb{R}^d)$ with the positive constant $G_d = \frac{d}{d+2} \left(\frac{2}{d+2}\right)^{2/d} (L_d^1)^{-2/d}$.

Proof. To obtain (4.37), note that by GNS (4.20) and Hölder we have that for any L^2 -normalized $\psi \in H^1(\mathbb{R}^d)$

$$\begin{aligned} \mathcal{E}[\psi] &\geq G_d \int_{\mathbb{R}^d} |\psi|^{2(1+2/d)} - \left(\int_{\mathbb{R}^d} |V_-|^{(d+2)/2} \right)^{2/(d+2)} \left(\int_{\mathbb{R}^d} |\psi|^{2(d+2)/d} \right)^{d/(d+2)} \\ &\geq -L_d^1 \int_{\mathbb{R}^d} |V_-|^{(d+2)/2}, \end{aligned}$$

where we used the fact that the function $\mathbb{R}_+ \ni t \mapsto At - Bt^{d/(d+2)}$ for $A, B > 0$ has the minimal value $-\frac{2}{d+2} \left(\frac{d}{d+2}\right)^{d/2} A^{-d/2} B^{(d+2)/2}$.

On the other hand, if (4.37) holds, then assume first that $\psi \in H^1(\mathbb{R}^d)$ with $\|\psi\|_2 = 1$ and let us write for an arbitrary potential V :

$$T[\psi] = T[\psi] + V[\psi] - V[\psi] \geq E_0 - \int_{\mathbb{R}^d} V|\psi|^2 \geq -L_d^1 \int_{\mathbb{R}^d} |V_-|^{1+d/2} - \int_{\mathbb{R}^d} V|\psi|^2.$$

Now, take $V(\mathbf{x}) := -c|\psi(\mathbf{x})|^\alpha$ and choose α such that the above integrals involving $|\psi|$ match modulo constants, i.e. $\alpha(1 + d/2) = \alpha + 2$, or equivalently, $\alpha = 4/d$. Thus,

$$T[\psi] \geq \left(c - c^{1+d/2} L_d^1\right) \int_{\mathbb{R}^d} |\psi|^{2(1+2/d)},$$

and we may finally optimize in $c > 0$ to obtain (4.20) with the claimed relationship between G_d and L_d^1 . Finally, the homogeneous GNS inequality (4.20) is obtained by simple rescaling $\psi = \lambda \tilde{\psi}$, in the case that $\lambda := \|\psi\|_2 \neq 1$. \square

Exercise 4.18. Prove Theorem 4.18 in the case $d = 1$ and $d = 2$.

Exercise 4.19. Prove that $E_0 > -\infty$ for (4.36).

4.6. Poincaré. The Heisenberg, Hardy and Sobolev inequalities were all *global* in the sense that they involved the full configuration space \mathbb{R}^n (or Dirichlet restrictions of it, by simple restriction of the domain to $H_0^1(\Omega) \subseteq H^1(\mathbb{R}^n)$). We shall now consider some *local* formulations of uncertainty principles (amounting to Neumann restrictions which potentially *increase* the domain), the prime example being the Poincaré inequality.

Definition 4.20 (Poincaré inequality). A **Poincaré inequality** on a domain $\Omega \subseteq \mathbb{R}^n$ with finite measure $|\Omega|$ is a lower bound of the form

$$\int_{\Omega} |\nabla u|^2 \geq C_P \int_{\Omega} |u - u_{\Omega}|^2 \quad (4.38)$$

for some constant $C_P = C_P(\Omega) > 0$ and for all $u \in H^1(\Omega)$, where in the r.h.s. we have subtracted the average of u on Ω ,

$$u_{\Omega} := |\Omega|^{-1} \int_{\Omega} u. \quad (4.39)$$

Remark 4.21. Note that if $C_P > 0$ then $\Omega \subseteq \mathbb{R}^d$ has to be a connected set, for otherwise we may choose u to be a non-zero constant on each connected component and such that $u_{\Omega} = 0$, for example $u = |\Omega_1|^{-1} \mathbf{1}_{\Omega_1} - |\Omega_2|^{-1} \mathbf{1}_{\Omega_2}$, so that the l.h.s. of (4.38) is zero but the r.h.s. non-zero. Also note that by dimensional scaling, $C_P(\Omega) = |\Omega|^{-2/d} C_P(\Omega/|\Omega|)$, where $C_P(\Omega/|\Omega|)$ only depends on the shape of Ω .

It is useful to reformulate the inequality (4.38) as an operator relation for the Laplacian on Ω . We note that, since $\nabla u_\Omega = 0$, the l.h.s. of (4.38) can also be written

$$\int_{\Omega} |\nabla u|^2 = \int_{\Omega} |\nabla(u - u_\Omega)|^2 = \langle (u - u_\Omega), -\Delta_{\Omega}^{\mathcal{N}}(u - u_\Omega) \rangle$$

and, with $u_0 := |\Omega|^{-1/2}$ the L^2 -normalized zero-eigenfunction of the Neumann Laplacian on Ω , we can write $u_\Omega = u_0 \langle u_0, u \rangle$, and thus

$$\langle u_0, u - u_\Omega \rangle = \langle u_0, u \rangle - \langle u_0, u_0 \rangle \langle u_0, u \rangle = 0.$$

In other words, if we introduce $P_0 := u_0 \langle u_0, \cdot \rangle$ the orthogonal projection operator on the ground-state eigenspace $W_0 = \mathbb{C}u_0$ and $P_0^\perp = \mathbb{1} - P_0$ the projection on the orthogonal subspace W_0^\perp , we have $u_\Omega = P_0 u$ and $u - u_\Omega = P_0^\perp u$. Hence, the Poincaré inequality (4.38) equivalently says

$$\langle P_0^\perp u, (-\Delta_{\Omega}^{\mathcal{N}}) P_0^\perp u \rangle \geq C_P \langle P_0^\perp u, P_0^\perp u \rangle$$

or, as an operator inequality,

$$(-\Delta_{\Omega}^{\mathcal{N}}) P_0^\perp \geq C_P P_0^\perp.$$

Hence, we see that finding the best possible constant C_P for a given domain Ω is the same as finding the second lowest eigenvalue $\lambda_1 \geq \lambda_0 = 0$ for the Laplace operator $-\Delta_{\Omega}^{\mathcal{N}}$ (with Neumann boundary conditions) on Ω ,

$$-\Delta_{\Omega}^{\mathcal{N}} = \sum_{k=0}^{\infty} \lambda_k P_k, \quad P_0 = u_0 \langle u_0, \cdot \rangle, \quad P_0^\perp = \sum_{k \geq 1} P_k = \sum_{k \geq 1} u_k \langle u_k, \cdot \rangle.$$

This is actually just the content of the min-max theorem of Section 2.5.1, applied to the form (4.38). Also, we see that $C_P = \lambda_1 - \lambda_0 > 0$ if and only if there is a gap in the spectrum between the lowest eigenvalue $\lambda_0 = 0$ (the ground-state energy) and the second-lowest one (the first excited energy level) λ_1 .

Example 4.22. As a prototype case one may consider the Laplacian on the unit interval $[0, 1]$. The eigenfunctions of the Neumann problem are $u_k(x) = C \cos(\pi k x)$ with eigenvalues $\lambda = \pi^2 k^2$, $k = 0, 1, 2, \dots$. Hence we have a Poincaré inequality

$$\int_0^1 |u'|^2 \geq \pi^2 \int_0^1 \left| u - \int_0^1 u \right|^2,$$

for $u \in H^1([0, 1])$, with the optimal Poincaré constant $C_P = \pi^2$. In the case of the Dirichlet problem, with $u_k(x) = C \sin(\pi k x)$, $\lambda = \pi^2 k^2$, $k = 1, 2, \dots$, one has an inequality

$$\int_0^1 |u'|^2 \geq \pi^2 \int_0^1 |u|^2,$$

for any $u \in H_0^1([0, 1])$, without any projection in this case.

Example 4.23. A Poincaré inequality of the form (4.38) cannot hold on the unbounded interval \mathbb{R} or \mathbb{R}_+ , not only because of the lack of an integrable ground state u_0 to project out as in (4.39), but more crucially because of the lack of a spectral gap in this case. We

have already seen and used that $\sigma(-\Delta_{\mathbb{R}}) = \sigma(\hat{p}_1^2) = [0, \infty)$, but also on the half-line \mathbb{R}_+ one may consider a sequence of trial states such as

$$u_L(x) = \sqrt{2/L} \sin(\pi x/L) \mathbf{1}_{[0,L]} \in H_0^1(\mathbb{R}_+) \subseteq H^1(\mathbb{R}_+).$$

By taking $L \rightarrow \infty$, such states have an arbitrarily low energy, and one may furthermore pick an orthogonal sequence such as $\{u_L(\cdot + nL)\}_{n=0,1,2,\dots}$ and use the min-max principle to find that the essential spectrum $\sigma_{\text{ess}}(-\Delta_{\mathbb{R}_+}^{N/D})$ starts at zero (such a sequence is known as a **Weyl sequence**). Furthermore, by e.g. multiplying u_L with a phase $e^{i\kappa x}$, any $\lambda = \kappa^2 \geq 0$ may be seen to be a point of the essential spectrum as well, so $\sigma(-\Delta_{\mathbb{R}_+}^{N/D}) = [0, \infty)$.

Note that the existence of a gap in the spectrum of the Laplacian on a domain Ω can also be interpreted as a form of the uncertainty principle of \hat{x}_j and \hat{p}_j , since the corresponding Hamiltonian describing the free kinetic energy of a particle on Ω of mass $m = 1/2$ is actually $\hat{H} = \hat{\mathbf{p}}_{\Omega}^2 = \hbar^2(-\Delta_{\Omega})$, which then has a gap of size proportional to \hbar^2 . If \hat{x}_j and \hat{p}_j would be made to commute, as they do classically, by formally taking $\hbar \rightarrow 0$ in (3.18), then

$$\sigma(\hat{H}) = \hbar^2 \{\lambda_0, \lambda_1, \dots\} \rightarrow [0, \infty)$$

and the gap would therefore close⁽¹⁷⁾. Another way to think about this limit is that \hbar may be compensated for by rescaling the domain, $\Omega \mapsto \Omega/\hbar$, and $\Omega/\hbar \rightarrow \mathbb{R}^d$ as $\hbar \rightarrow 0$, so that

$$\sigma(\hat{H}) = \sigma(-\Delta_{\Omega/\hbar}) \xrightarrow{\hbar \rightarrow 0} \sigma(-\Delta_{\mathbb{R}^d}) = \sigma(\hat{\mathbf{p}}_{\mathbb{R}^d}^2) = \sigma(\check{\mathbf{p}}_{\mathbb{R}^d}^2) = [0, \infty),$$

by Fourier transform.

Example 4.24. Poincaré inequalities also extend to other contexts where there is a gap in the spectrum, such as on compact, connected manifolds. One has for example the following Poincaré inequality on the unit sphere \mathbb{S}^{d-1} in \mathbb{R}^d :

$$\int_{\mathbb{S}^{d-1}} |\nabla u|^2 \geq (d-1) \int_{\mathbb{S}^{d-1}} \left| u - |\mathbb{S}^{d-1}|^{-1} \int_{\mathbb{S}^{d-1}} u \right|^2, \quad (4.40)$$

for $u \in H^1(\mathbb{S}^{d-1})$. This follows from the following theorem concerning the spectrum of the **Laplace-Beltrami operator** on \mathbb{S}^{d-1} , i.e. the operator $-\Delta_{\mathbb{S}^{d-1}}$ associated to the non-negative quadratic form of the l.h.s. of (4.40) (see e.g. [Shu01, Chapter 22] for further details and proofs).

Theorem 4.25 (Spectrum of the Laplacian on the sphere; see e.g. [Shu01, Theorem 22.1 and Corollary 22.2]). *The spectrum of the operator $-\Delta_{\mathbb{S}^{d-1}}$ is discrete and its eigenvalues are given by $\lambda = k(k+d-2)$, $k = 0, 1, 2, \dots$, with multiplicity given by the dimension of the space of homogeneous, harmonic polynomials on \mathbb{R}^d of degree k , which is $\binom{k+d-1}{d-1} - \binom{k+d-3}{d-1}$ for $k \geq 2$ (and 1 for $k = 0$ respectively d for $k = 1$).*

Exercise 4.20. *Prove the Poincaré inequality (4.40) on the unit circle \mathbb{S}^1 , by treating it as an interval $[0, 2\pi]$ with periodic boundary conditions, $u(0) = u(2\pi)$, $u'(0) = u'(2\pi)$.*

Exercise 4.21. *Prove a Poincaré inequality on an annulus $\Omega_{R_1, R_2} = B_{R_2}(0) \setminus \bar{B}_{R_1}(0)$ and give some explicit non-zero lower bound for the constant C_P depending on $R_2 > R_1 > 0$.*

⁽¹⁷⁾In fact any gap in the spectrum will close in this limit because the eigenvalues λ_k are distributed rather uniformly; they can on bounded regular domains Ω be shown to satisfy $(\lambda_{k+1} - \lambda_k)/\lambda_{k+1} \rightarrow 0$ as $k \rightarrow \infty$ (cf. Exercise 5.2).

4.7. Local Sobolev-type inequalities. There is a family of important inequalities which combine the properties of the global Sobolev inequality of Section 4.3 with the local properties of the Poincaré inequality of Section 4.6, and which are thus called **Poincaré-Sobolev inequalities**. However, these are typically a little more involved to prove and we shall therefore instead take a more direct route to obtain the inequalities that we will need, of the form of the Gagliardo-Nirenberg-Sobolev inequalities of Theorems 4.14 and 4.16, and which only relies on knowledge of the eigenvalues for the Laplacian on a cube Q . They could be considered variants of the above-mentioned Poincaré-Sobolev inequalities though. See [BVV18b, BVV18a] for very recent generalizations and improvements of the bounds given below.

4.7.1. Laplacian eigenvalues on the cube. Consider the Neumann Laplacian on a cube $Q = [0, L]^d \subseteq \mathbb{R}^d$ and the number $N(E)$ of its eigenvalues λ_k , ordered according to their multiplicity, below an energy $E > 0$ (note that since $\lambda_0 = 0$ we always have $N(E) \geq 1$). In the case $d = 1$,

$$\lambda_k = \frac{\pi^2}{|Q|^2} k^2, \quad k = 0, 1, 2, \dots,$$

and

$$N(E) - 1 = \#\{k : 0 < \lambda_k < E\} = \#\{k \in \mathbb{Z} : 0 < k < E^{1/2}|Q|/\pi\} \leq E^{1/2}|Q|/\pi.$$

In the case $d \geq 2$ we have

$$\lambda_{\mathbf{k}} = \frac{\pi^2}{|Q|^{2/d}} |\mathbf{k}|^2, \quad \mathbf{k} \in \mathbb{Z}_{\geq 0}^d,$$

and

$$\begin{aligned} N(E) - 1 &= \#\{\mathbf{k} : 0 < \lambda_{\mathbf{k}} < E\} = \#\{\mathbf{k} \in \mathbb{Z}_{\geq 0}^d : 0 < |\mathbf{k}| < E^{1/2}|Q|^{1/d}/\pi\} \\ &\leq 2^d (E^{1/2}|Q|^{1/d}/\pi)^d, \end{aligned}$$

where we for $E^{1/2}|Q|^{1/d}/\pi \geq 1$ (otherwise it is zero) very roughly bounded the number of integer points of the first quadrant inside a sphere of radius R by the volume of an enclosing cube of side length $R + 1 \leq 2R$. Hence, as a uniform bound

$$N(E) \leq 1 + 2^d |Q|/\pi^d \cdot E^{d/2} \tag{4.41}$$

for all $d \geq 1$. Also note that the orthonormal eigenfunctions are given explicitly by

$$u_{\mathbf{k}}(\mathbf{x}) = |Q|^{-1/2} \prod_{j=1}^d c_{k_j} \cos \frac{\pi k_j x_j}{|Q|^{1/d}},$$

with $c_0 = 1$ and $c_{k \geq 1} = \sqrt{2}$, so that

$$\|u_{\mathbf{k}}\|_{\infty} \leq |Q|^{-1/2} \prod_{j=1}^d c_{k_j} \leq 2^{d/2} |Q|^{-1/2}. \tag{4.42}$$

4.7.2. *Poincaré-Sobolev-type bound.* The following is a local version of the Gagliardo–Nirenberg–Sobolev inequality of Theorem 4.14 (it was given in this form as Theorem 13 in [LS13a]):

Theorem 4.26. *For any $d \geq 1$ there exists a constant $C_d > 0$ such that for any d -cube $Q \subseteq \mathbb{R}^d$ and every $u \in H^1(Q)$*

$$\int_Q |\nabla u|^2 \geq C_d \left(\int_Q |u|^2 \right)^{-2/d} \int_Q \left[|u| - \left(\frac{\int_Q |u|^2}{|Q|} \right)^{1/2} \right]_+^{2(1+2/d)}.$$

Proof. We make a decomposition of u similar to the one in the proof of Theorem 4.14, but this time w.r.t. the Neumann kinetic energy on Q . Namely, we define $u = u_{E,-} + u_{E,+}$ with an energy cut-off $E > 0$ and the spectral projections

$$u_{E,-} := P_{[0,E]}^{-\Delta_Q^N} u \quad \text{and} \quad u_{E,+} := P_{[E,\infty)}^{-\Delta_Q^N} u.$$

In this case we have by the spectral theorem and the properties of the projection-valued measures that

$$\int_0^\infty \|u_{E,+}\|_2^2 dE = \int_0^\infty \left\langle u, P_{[E,\infty)}^{-\Delta_Q^N} u \right\rangle dE = \left\langle u, -\Delta_Q^N u \right\rangle,$$

since $P_{[E,\infty)}^A = \int_{\mathbb{R}} \mathbb{1}_{\{\lambda \geq E\}} dP^A(\lambda)$ and thus $\int_0^\infty P_{[E,\infty)}^A dE = \int_{\mathbb{R}} \lambda dP^A(\lambda) = A$ for any self-adjoint operator A (a reader worried about such formal manipulation may note that it is applied here in the form sense with non-negative integrands).

Let us denote the eigenvalues and orthonormal eigenfunctions of $-\Delta_Q^N$, ordered according to their multiplicity, as usual by $\{\lambda_k\}_{k=0}^\infty$ and $\{u_k\}_{k=0}^\infty$. For the low-energy part we have then for each $\mathbf{x} \in Q$

$$\begin{aligned} |u_{E,-}(\mathbf{x})|^2 &= \left| P_{[0,E]}^{-\Delta_Q^N} u(\mathbf{x}) \right|^2 = \left| \sum_{\lambda_k < E} \langle u_k, u \rangle u_k(\mathbf{x}) \right|^2 = \left| \left\langle \sum_{\lambda_k < E} \overline{u_k(\mathbf{x})} u_k, u \right\rangle \right|^2 \\ &\leq \left(\sum_{\lambda_k < E} |u_k(\mathbf{x})|^2 \right) \|u\|_2^2, \end{aligned}$$

by Cauchy–Schwarz and the orthonormality of $\{u_k\}$. Furthermore, by (4.41) and (4.42), we have that

$$\sum_{\lambda_k < E} |u_k(\mathbf{x})|^2 \leq \frac{1}{|Q|} + \sum_{0 < \lambda_k < E} \frac{2^d}{|Q|} \leq \frac{1}{|Q|} + \frac{2^{2d}}{\pi^d} E^{d/2}.$$

After these preparations we may finally use the triangle inequality (4.24) and the integral identity (4.25) to obtain

$$\begin{aligned}
\int_Q |\nabla u|^2 &= \int_Q \int_0^\infty |u_{E,+}(\mathbf{x})|^2 dE d\mathbf{x} \\
&\geq \int_Q \int_0^\infty \left[|u(\mathbf{x})| - \left(|Q|^{-1} + 2^{2d} \pi^{-d} E^{d/2} \right)^{1/2} \|u\|_2 \right]_+^2 dE d\mathbf{x} \\
&\geq \int_Q \int_0^\infty \left[|u(\mathbf{x})| - |Q|^{-1/2} \|u\|_2 - 2^d \pi^{-d/2} \|u\|_2 E^{d/4} \right]_+^2 dE d\mathbf{x} \\
&= C_d \|u\|_2^{-4/d} \int_Q \left[|u(\mathbf{x})| - |Q|^{-1/2} \|u\|_2 \right]_+^{2(1+2/d)} d\mathbf{x},
\end{aligned}$$

with $C_d = d^2(2^{-4}\pi^2)/((d+2)(d+4))$. \square

Exercise 4.22 (Suggested by Rafael Benguria). *Prove a corresponding local GNS inequality on the interval $[-1/2, 1/2]$ on the subspace of odd functions. By how much would you expect the optimal constant to improve in this case?*

4.8. Local uncertainty and density formulations. We finish this chapter on uncertainty principles with some local many-body formulations involving the one-body density ϱ_Ψ . These will in later chapters be supplemented with local formulations of the exclusion principle to prove powerful global kinetic energy inequalities of wide applicability.

The following is a local version of the many-body GNS inequality of Theorem 4.16 (it was given in this form as Theorem 14 in [LS13a]):

Theorem 4.27. *For any $d \geq 1$ there exists a constant $C_d > 0$ (same as in Theorem 4.26) such that for any d -cube $Q \subseteq \mathbb{R}^d$, all $N \geq 1$, and L^2 -normalized $\Psi \in H^1(\mathbb{R}^{dN})$*

$$\sum_{j=1}^N \int_{\mathbb{R}^{dN}} |\nabla_j \Psi|^2 \mathbf{1}_Q(\mathbf{x}_j) d\mathbf{x} \geq C_d \left(\int_Q \varrho_\Psi \right)^{-2/d} \int_Q \left[\varrho_\Psi^{1/2} - \left(\frac{\int_Q \varrho_\Psi}{|Q|} \right)^{1/2} \right]_+^{2(1+2/d)}.$$

The proof is a straightforward modification of the one-body Theorem 4.26, using

$$\sum_{j=1}^N \int_{\mathbb{R}^{dN}} |\nabla_j \Psi|^2 \mathbf{1}_Q(\mathbf{x}_j) d\mathbf{x} = \sum_{j=1}^N \int_{\mathbb{R}^{d(N-1)}} \int_Q |\nabla_j \Psi|^2 d\mathbf{x}_j d\mathbf{x}' = \sum_{j=1}^N \int_{\mathbb{R}^{d(N-1)}} \int_0^\infty \|u_j^{E,+}\|^2 dE$$

as in Exercise 4.13, with $\int_{\mathbb{R}^{d(N-1)}} \sum_{j=1}^N |u_j(\mathbf{x}, \mathbf{x}')|^2 d\mathbf{x}' = \varrho_\Psi(\mathbf{x})$ and

$$\int_{\mathbb{R}^{d(N-1)}} \sum_{j=1}^N |u_j^{E,-}(\mathbf{x}, \mathbf{x}')|^2 d\mathbf{x}' \leq \left(\frac{1}{|Q|} + \frac{2^{2d}}{\pi^d} E^{d/2} \right) \int_{\mathbb{R}^{d(N-1)}} \sum_{j=1}^N \|u_j(\cdot, \mathbf{x}')\|_{L^2(Q)}^2 d\mathbf{x}'.$$

Similarly as in the global case, one could alternatively have used a local version of the Hoffmann-Ostenhof inequality (cf. Lemma 4.17) together with Theorem 4.26 directly.

Now, let us write for the total expected kinetic energy of an N -body wave function $\Psi \in H^1(\mathbb{R}^{dN})$

$$T[\Psi] = \langle \hat{T} \rangle_\Psi = \int_{\mathbb{R}^{dN}} |\nabla \Psi|^2.$$

We also introduce the **local expected kinetic energy** on the cube $Q \subseteq \mathbb{R}^d$ (which may of course also be replaced by a general subdomain Ω)

$$T^Q[\Psi] := \sum_{j=1}^N \int_{\mathbb{R}^{dN}} |\nabla_j \Psi|^2 \mathbf{1}_Q(\mathbf{x}_j) dx = \sum_{j=1}^N \|\mathbf{1}_{\mathbf{x}_j \in Q} \hat{\mathbf{p}}_j \Psi\|^2.$$

Using the above inequality we may obtain a bound for this quantity of the particularly convenient form

$$T^Q[\Psi] \geq C_1 \frac{\int_Q \varrho_\Psi^{1+2/d}}{(\int_Q \varrho_\Psi)^{2/d}} - C_2 \frac{\int_Q \varrho_\Psi}{|Q|^{2/d}},$$

for some constants $C_1, C_2 > 0$, which we shall refer to as a **local uncertainty principle**.

Lemma 4.28 (Local uncertainty principle). *For any d -cube Q and any $\varepsilon \in (0, 1)$ we have*

$$T^Q[\Psi] \geq C_d \varepsilon^{1+4/d} \frac{\int_Q \varrho_\Psi^{1+2/d}}{(\int_Q \varrho_\Psi)^{2/d}} - C_d \left(1 + \left(\frac{\varepsilon}{1-\varepsilon} \right)^{1+4/d} \right) \frac{\int_Q \varrho_\Psi}{|Q|^{2/d}}, \quad (4.43)$$

with C_d as in Theorems 4.26 and 4.27.

Proof. By Theorem 4.27 we have that

$$T^Q[\Psi] \geq \frac{C_d}{(\int_Q \varrho_\Psi)^{2/d}} \int_Q \left[\varrho_\Psi(\mathbf{x})^{\frac{1}{2}} - \left(\frac{\int_Q \varrho_\Psi}{|Q|} \right)^{\frac{1}{2}} \right]_+^{2+4/d} d\mathbf{x},$$

with

$$\begin{aligned} & \int_Q \left[\varrho_\Psi(\mathbf{x})^{\frac{1}{2}} - \left(\frac{\int_Q \varrho_\Psi}{|Q|} \right)^{\frac{1}{2}} \right]_+^{2+4/d} d\mathbf{x} \\ & \geq \int_Q \left| \varrho_\Psi(\mathbf{x})^{\frac{1}{2}} - \left(\frac{\int_Q \varrho_\Psi}{|Q|} \right)^{\frac{1}{2}} \right|^{2+4/d} d\mathbf{x} - \int_Q \left(\frac{\int_Q \varrho_\Psi}{|Q|} \right)^{1+2/d} \\ & = \left\| \varrho_\Psi^{\frac{1}{2}} - \left(\frac{\int_Q \varrho_\Psi}{|Q|} \right)^{\frac{1}{2}} \right\|_{2+4/d}^{2+4/d} - \frac{(\int_Q \varrho_\Psi)^{1+2/d}}{|Q|^{2/d}}. \end{aligned}$$

The first term is bounded below by

$$\left(\|\varrho_\Psi^{\frac{1}{2}}\|_{2+4/d} - \left\| \left(\frac{\int_Q \varrho_\Psi}{|Q|} \right)^{\frac{1}{2}} \right\|_{2+4/d} \right)^{2+4/d}$$

using the triangle inequality on $L^p(Q)$. Furthermore, by convexity of the function $t \mapsto t^p$ for $t \geq 0$, $p \geq 1$ we have for any $a, b \geq 0$ and $\varepsilon \in (0, 1)$ that

$$\varepsilon a^p + (1-\varepsilon)b^p \geq (\varepsilon a + (1-\varepsilon)b)^p,$$

and hence with $a = A - B$ and $b = \frac{\varepsilon}{1-\varepsilon}B$,

$$(A - B)^p \geq \varepsilon^{p-1} A^p - \left(\frac{\varepsilon}{1-\varepsilon} \right)^{p-1} B^p.$$

Applying this inequality to the norms above with $p = 2 + 4/d$, we finally arrive at (4.43). \square

Finally, given a partition \mathcal{P} of the one-particle configuration space \mathbb{R}^d into disjoint cubes,

$$\mathbb{R}^d = \bigcup_{Q \in \mathcal{P}} \bar{Q}, \quad Q \cap Q' = \emptyset \quad \forall Q, Q' \in \mathcal{P} \text{ s.t. } Q \neq Q',$$

we have, with $\mathbf{1} = \sum_{Q \in \mathcal{P}} \mathbf{1}_Q$, that

$$T[\Psi] = \sum_{Q \in \mathcal{P}} T^Q[\Psi] \geq \sum_{Q \in \mathcal{P}} \left(C_1 \frac{\int_Q \varrho_\Psi^{1+2/d}}{(\int_Q \varrho_\Psi)^{2/d}} - C_2 \frac{\int_Q \varrho_\Psi}{|Q|^{2/d}} \right). \quad (4.44)$$

This bound for the total expected kinetic energy of Ψ can only be useful if the positive terms are stronger than the negative ones, in other words, if the expected number of particles $\sum_{j=1}^N \langle \mathbf{1}_{\mathbf{x}_j \in Q} \rangle_\Psi = \int_Q \varrho_\Psi$ on each cube Q is not too large, *and* if the density is sufficiently localized on Q ,

$$\frac{1}{|Q|} \int_Q \varrho_\Psi^{1+2/d} \gg \left(\frac{1}{|Q|} \int_Q \varrho_\Psi \right)^{1+2/d}.$$

For the case of rather homogeneous density distributions the above inequality fails, and the local uncertainty principle (4.44) will for example have to be supplemented with an exclusion principle in order to yield a non-trivial global bound. This will be the topic of the next section.

5. EXCLUSION PRINCIPLES

In this section we consider consequences of the theory for identical particles and exchange phases that was outlined in Section 3.7, as well as related concepts, both locally and globally on the configuration space.

Recall that in general we have a division of the full N -particle Hilbert space $\mathcal{H} \cong \bigotimes^N \mathfrak{H}$ of distinguishable particles into subspaces of symmetric (**bosonic**) respectively antisymmetric (**fermionic**) states of *indistinguishable* particles,

$$\mathcal{H}_{\text{sym}} \cong \bigotimes_{\text{sym}}^N \mathfrak{H}, \quad \mathcal{H}_{\text{asym}} \cong \bigwedge^N \mathfrak{H},$$

where \mathfrak{H} denotes the one-particle Hilbert space. For illustration let us consider here the usual space $\mathfrak{H} = L^2(\mathbb{R}^d)$ of a particle in \mathbb{R}^d , but other spaces will be of interest as well. When acting with the non-interacting N -body Hamiltonian operator (as given e.g. in (3.36))

$$\hat{H} = \sum_{j=1}^N \hat{h}_j, \quad \hat{h}_j = \hat{h}(\hat{\mathbf{x}}_j, \hat{\mathbf{p}}_j) = -\Delta_{\mathbf{x}_j} + V(\mathbf{x}_j) \in \mathcal{L}(\mathfrak{H}),$$

on \mathcal{H}_{sym} respectively $\mathcal{H}_{\text{asym}}$, we may observe a crucial difference in the resulting spectra. Namely, let us assume for simplicity that we can diagonalize the one-body operator \hat{h} into a complete discrete set of real eigenvalues $\sigma(\hat{h}) = \{\lambda_n\}_{n=0}^{\infty}$ and a corresponding basis of orthonormal one-body eigenstates $\{u_n\}_{n=0}^{\infty}$ in \mathfrak{H} , with an ordering $\lambda_0 \leq \lambda_1 \leq \dots$ according to multiplicity. Then the corresponding N -body eigenstates $\Psi \in \mathcal{H}$ of \hat{H} are simply the tensor products

$$\Psi = \Psi_{\{n_j\}} := u_{n_1} \otimes u_{n_2} \otimes \dots \otimes u_{n_N}, \quad n_j \in \mathbb{N}_0, \quad (5.1)$$

with

$$\hat{H}\Psi_{\{n_j\}} = \sum_{j=1}^N u_{n_1} \otimes \dots \otimes \hat{h}u_{n_j} \otimes \dots \otimes u_{n_N} = \sum_{j=1}^N \lambda_{n_j} \Psi_{\{n_j\}}.$$

In other words, the N -body energy eigenvalues in the case of distinguishable particles are

$$E_{\{n_j\}} = \sum_{j=1}^N \lambda_{n_j}, \quad \{n_j\} \in \mathbb{N}_0^N.$$

However, with the symmetry restriction in $\mathcal{H}_{\text{asym}}$, the basis (5.1) reduces to the antisymmetric product (also known as a **Slater determinant**)

$$\Psi_{\text{asym}} = u_{n_1} \wedge u_{n_2} \wedge \dots \wedge u_{n_N} := \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \text{sign}(\sigma) u_{\sigma(n_1)} \otimes u_{\sigma(n_2)} \otimes \dots \otimes u_{\sigma(n_N)},$$

with $n_1 < n_2 < \dots < n_N$. Because of the antisymmetry we cannot use the same one-body state u_n more than once in the expression, namely $u_n \wedge u_n = 0$, and this symmetry restriction is known in physics as the **Pauli principle** and is thus obeyed by fermions, such as the electrons of an atom [Pau47].

On the other hand, in a basis of the bosonic space \mathcal{H}_{sym} we must take symmetric tensor products, and for example the following state is allowed:

$$\Psi_{\text{sym}} = \bigotimes^N u_0 := u_0 \otimes u_0 \otimes \dots \otimes u_0 \quad (N \text{ factors}),$$

that is $\Psi_{\text{sym}}(\mathbf{x}) = \prod_{j=1}^N u_0(\mathbf{x}_j)$, with u_0 corresponding to the lowest eigenvalue λ_0 of \hat{h} . This will in fact be the ground state of \hat{H} (both when considered as an operator on \mathcal{H} and on \mathcal{H}_{sym} , but *not* on $\mathcal{H}_{\text{asym}}$ \nexists Ψ_{sym}). Namely, we note that the energy eigenvalue of this state Ψ_{sym} is

$$E_{0,\text{sym}}(N) = N\lambda_0 \leq \sum_{j=1}^N \lambda_{n_j} = E_{\{n_j\}},$$

for any multi-index $\{n_j\} \in \mathbb{N}_0^N$, and hence this is the ground-state energy. In contrast, on states Ψ_{asym} we necessarily obtain a sum of higher and higher energies, and the smallest possible value is

$$E_{0,\text{asym}}(N) = \sum_{k=0}^{N-1} \lambda_k \leq \sum_{j=1}^N \lambda_{n_j} = E_{\{n_j\}}, \quad (5.2)$$

for any admissible $\{n_j\}$, i.e. $n_1 < n_2 < \dots < n_N$. Because of this symmetry restriction the fermionic g.s. energy must (unless the lowest eigenvalue λ_0 is infinitely degenerate) be strictly larger than the bosonic (or the distinguishable) one for large enough N , and in realistic systems with finite degeneracies it will actually be *significantly* larger as $N \rightarrow \infty$.

These differences in the rules for distributing bosons and fermions into one-body states, enforced by the Pauli principle, has remarkable macroscopic consequences as one considers large ensembles of particles, which is the aim of **quantum statistical mechanics**. Bosons are then said to obey **Bose–Einstein statistics** while fermions are subject to **Fermi–Dirac statistics**. Distinguishable particles on the other hand obey **Maxwell–Boltzmann statistics** and are sometimes called **boltzons**.

We shall in this chapter also consider exclusion principles in a more general context. In particular, we allow for a weakening of the above Pauli principle — which is actually relevant for real fermions appearing in nature such as electrons with spin — and we also extend the notion of the exclusion of points in the many-body configuration space to encompass other important cases such as bosons subject to repulsive pair interactions, as well as anyons in two dimensions. The relatively straightforward generalization of quantum statistics to allow for several particles in each one-body state (beyond spin) has a long history, going back at least to Gentile [Gen40, Gen42] and is thus known as **Gentile statistics** or **intermediate (exclusion) statistics**. More recent and less trivial generalizations of such concepts have been reviewed in [Hal91, Isa94, Wu94, Myr99, Pol99, Kha05].

Exercise 5.1. Compute the ground-state energy $E_{0,\text{asym}}$ for N fermions in a harmonic trap $V_{\text{osc}}(\mathbf{x}) = \frac{1}{2}m\omega^2|\mathbf{x}|^2$ in $d = 1$ and in $d = 2$ (see Example 3.16). Note that in the latter case there are certain “magic numbers” $N = n(n+1)/2$, $n \in \mathbb{N}$, such that

$$E_{0,\text{asym}}(N) = (1 + 2^2 + \dots + n^2)\hbar\omega = \frac{1}{3}N\sqrt{8N+1}\hbar\omega.$$

Exercise 5.2. Consider N fermions in a cube $Q \subseteq \mathbb{R}^d$. Use the values in Section 4.7.1 and an integral approximation of a Riemann sum to show that, as a leading-order approximation,

$$E_{0,\text{asym}}(N) = \sum_{k=0}^{N-1} \lambda_k(-\Delta_Q^{\mathcal{N}/\mathcal{D}}) \approx K_d^{\text{cl}} \frac{N^{1+2/d}}{|Q|^{2/d}}, \quad K_d^{\text{cl}} := 4\pi \frac{d}{d+2} \left(\frac{2}{d+2} \right)^{\frac{2}{d}} \Gamma \left(2 + \frac{d}{2} \right)^{\frac{2}{d}}. \quad (5.3)$$

This is known as **Weyl's asymptotic formula** for the sum of eigenvalues, and it thus determines the g.s. energy of a **free Fermi gas** confined to a box, with the constants

$$K_1^{\text{cl}} = \frac{\pi^2}{3}, \quad K_2^{\text{cl}} = 2\pi, \quad K_3^{\text{cl}} = \frac{3}{5}(6\pi^2)^{\frac{2}{3}}.$$

Exercise 5.3. Compute an upper bound to $E_{0,\text{asym}}(N)$ of the correct order (5.3) in $d = 1, 2, 3$ by constructing a trial state Ψ_{asym} by localizing each particle to a separate cube, e.g. taking $u_j \in L^2(Q_j)$ to be Dirichlet ground states on the respective cubes Q_j , and then antisymmetrizing the full expression. Does one gain anything by localizing on balls instead? (Hint: the optimal packing density of circles is $\pi/(2\sqrt{3})$ and of spheres is $\pi/(3\sqrt{2})$.)

5.1. Fermions. Let us first consider some local consequences of the Pauli principle for fermions that will turn out to be particularly useful in our context of stability. We denote $H_{\text{asym}}^1 = H^1 \cap \mathcal{H}_{\text{asym}}$, and so on.

5.1.1. The Pauli principle. One has the following simple consequence of the Pauli principle for fermions on a cube Q :

Proposition 5.1. Let $Q \subseteq \mathbb{R}^d$ be a d -cube, $d \geq 1$. For any $N \geq 1$ and $\Psi \in H_{\text{asym}}^1(Q^N)$, we have

$$\int_{Q^N} |\nabla \Psi|^2 \geq (N-1) \frac{\pi^2}{|Q|^{2/d}} \int_{Q^N} |\Psi|^2. \quad (5.4)$$

Proof. Using the same argument of simple eigenvalue estimation as in (5.2), but now locally with the one-particle space $\mathfrak{H} = L^2(Q)$ and $0 \neq \Psi \in \bigwedge^N \mathfrak{H}$, we find in this case

$$\frac{\int_{Q^N} |\nabla \Psi|^2}{\int_{Q^N} |\Psi|^2} \geq E_0 \left(-\Delta_{Q^N} \Big|_{\bigwedge^N \mathfrak{H}} \right) = \sum_{k=0}^{N-1} \lambda_k(-\Delta_Q^N).$$

Now recall the energy levels λ_k of the Neumann Laplacian $-\Delta_Q^N$ given in Section 4.7.1:

$$\lambda_0 = 0 \quad (\text{here } \mathbf{k} = \mathbf{0}), \quad \lambda_{k \geq 1} \geq \lambda_1 = \frac{\pi^2}{|Q|^{2/d}} \quad (\text{here } |\mathbf{k}| \geq 1),$$

which proves the proposition. \square

The above bound gives a concrete local measure of the exclusion principle, as it tells us that, while a single particle may have zero energy on a finite domain (as is possible here due to the Neumann b.c.), as soon as there are two or more particles on the same domain, the energy must be strictly positive. However, if the particles were bosons or distinguishable then one could have chosen all particles to be in the ground state on the domain, i.e. the constant function, and thus obtained zero energy. The domain considered above was a cube but similar bounds are naturally valid on other domains as well, and in fact the corresponding bound on a ball (see (5.5) below) was used by Dyson and Lenard in their original proof of stability of fermionic matter [DL67, Lemma 5]. Indeed the only property of fermionic systems (compared to bosonic or boltzonic) used in their proof was this remarkably weak implication of the exclusion principle, with an energy which only grows *linearly* with N , as opposed to the true energy which grows much faster with N according to the Weyl asymptotics as we saw above (Exercise 5.2). This curious fact, that matter turns out to be stabilized sufficiently by the exclusion principle acting effectively

between pairs (and to a lesser extent triplets etc.) of neighboring electrons, was discussed briefly in [Dys68] and [Len73], and will be further clarified in the coming sections.

One may alternatively prove (5.4) resp. (5.5) directly via the Poincaré inequality on the domain; see [Len73, Theorem 8]. See also [LNP16, Lemma 11] for an extension of this type of exclusion bound to kinetic energy operators involving arbitrary powers of the momentum (even fractional, which is relevant for relativistic stability).

Exercise 5.4. *Prove a corresponding Pauli bound on a disk or a ball $B = B_R(0)$ of radius R , $\Psi \in H_{\text{asym}}^1(B^N)$,*

$$\int_{B^N} |\nabla \Psi|^2 \geq (N-1) \frac{\xi^2}{R^2} \int_{B^N} |\Psi|^2, \quad (5.5)$$

where for the two-dimensional disk, $\xi \approx 1.841$ denotes the first non-trivial zero of the derivative of the Bessel function J_1 , and for the three-dimensional ball, $\xi \approx 2.082$ denotes the smallest positive root x of the equation $\frac{d^2}{dx^2} \frac{\sin x}{x} = 0$. (Hint: You may use that the eigenvalue problem on the ball separates according to Theorem 4.25.)

5.1.2. *Fermionic uncertainty and statistical repulsion.* Another useful and concrete measure of the exclusion principle between fermions comes in the form of a strengthened uncertainty principle. Namely, as we shall see below, fermions turn out to satisfy an effective pairwise repulsion, and the corresponding mathematical statement may be referred to as a **fermionic many-body Hardy inequality**. Inequalities of this form were introduced in [HOHOLT08] in the global case, and were subsequently generalized to anyons in two dimensions and to local formulations in [LS13a, LL18]. The optimal constant in the inequality for fermions in the global case for $d \geq 3$ was also discussed in [FHOLS06]. We will here only discuss the simpler global case, although it is important to stress that the repulsion persists also locally, which is not the case with the usual Hardy inequality without antisymmetry.

Let us start with the following simple one-body version of the inequality (which has been pointed out already in [Bir61]):

Lemma 5.2 (One-body Hardy with antisymmetry). *If $u \in H^1(\mathbb{R}^d)$ is antipodal-antisymmetric, i.e. $u(-\mathbf{x}) = -u(\mathbf{x})$, then*

$$\int_{\mathbb{R}^d} |\nabla u(\mathbf{x})|^2 d\mathbf{x} \geq \frac{d^2}{4} \int_{\mathbb{R}^d} \frac{|u(\mathbf{x})|^2}{|\mathbf{x}|^2} d\mathbf{x}.$$

Remark 5.3. Note that this improves upon the constant of the standard Hardy inequality of Theorem 4.4 for $d \geq 2$, and that for $d = 1$ antisymmetry and continuity implies $u(0) = 0$ and hence $u \in H_0^1(\mathbb{R} \setminus \{0\})$, reducing therefore to the standard inequality.

Proof. We may write in terms of spherical coordinates $\mathbf{x} = \mathbf{x}(r, \omega)$, $r \geq 0$, $\omega \in \mathbb{S}^{d-1}$,

$$\int_{\mathbb{R}^d} |\nabla u(\mathbf{x})|^2 d\mathbf{x} = \int_{r=0}^{\infty} \int_{\mathbb{S}^{d-1}} \left(|\partial_r u|^2 + \frac{|\nabla_{\omega} u|^2}{r^2} \right) r^{d-1} dr d\omega \quad (5.6)$$

and change the order of integration by Fubini. The usual Hardy inequality (4.5) actually concerns the radial part here (exercise), namely for any $\omega \in \mathbb{S}^{d-1}$,

$$\int_0^{\infty} |\partial_r u(r, \omega)|^2 r^{d-1} dr \geq \frac{(d-2)^2}{4} \int_0^{\infty} \frac{|u(r, \omega)|^2}{r^2} r^{d-1} dr. \quad (5.7)$$

For the angular part of the derivative we may use the Poincaré inequality on \mathbb{S}^{d-1} given in (4.40),

$$\int_{\mathbb{S}^{d-1}} |\nabla_\omega u(r, \omega)|^2 d\omega \geq (d-1) \int_{\mathbb{S}^{d-1}} |u(r, \omega)|^2 d\omega, \quad (5.8)$$

since, by antipodal antisymmetry, $\int_{\mathbb{S}^{d-1}} u(r, \omega) d\omega = 0$ for all $r \geq 0$. The lemma then follows by combining these two inequalities. \square

By applying this lemma in pairwise relative coordinates, one obtains the following many-body Hardy inequality [HOHOLT08, Theorem 2.8]:

Theorem 5.4 (Many-body Hardy with antisymmetry). *If $\Psi \in H_{\text{asym}}^1(\mathbb{R}^{dN})$ then*

$$\int_{\mathbb{R}^{dN}} \sum_{j=1}^N |\nabla_j \Psi|^2 dx \geq \frac{d^2}{N} \int_{\mathbb{R}^{dN}} \sum_{1 \leq j < k \leq N} \frac{|\Psi(\mathbf{x})|^2}{|\mathbf{x}_j - \mathbf{x}_k|^2} dx + \frac{1}{N} \int_{\mathbb{R}^{dN}} \left| \sum_{j=1}^N \nabla_j \Psi \right|^2 dx. \quad (5.9)$$

Proof. We first use the many-body parallelogram identity (3.38)

$$\sum_{j=1}^N |\nabla_j \Psi|^2 = \frac{1}{N} \sum_{1 \leq j < k \leq N} |\nabla_j \Psi - \nabla_k \Psi|^2 + \frac{1}{N} \left| \sum_{j=1}^N \nabla_j \Psi \right|^2,$$

and then for each pair (j, k) of particles we introduce relative coordinates,

$$\mathbf{r}_{jk} := \mathbf{x}_j - \mathbf{x}_k, \quad \mathbf{X}_{jk} := \frac{1}{2}(\mathbf{x}_j + \mathbf{x}_k), \quad \nabla_{\mathbf{r}_{jk}} = \frac{1}{2}(\nabla_j - \nabla_k), \quad \nabla_{\mathbf{X}_{jk}} = \nabla_j + \nabla_k.$$

Thus, splitting the coordinates according to $\mathbf{x} = (\mathbf{x}_j, \mathbf{x}_k; \mathbf{x}')$, with $\mathbf{x}' \in \mathbb{R}^{d(N-2)}$ and $j < k$ fixed, we may define the relative function

$$u(\mathbf{r}, \mathbf{X}) := \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_j = \mathbf{X} + \frac{1}{2}\mathbf{r}, \dots, \mathbf{x}_k = \mathbf{X} - \frac{1}{2}\mathbf{r}, \dots, \mathbf{x}_N),$$

for which we have that $u(-\mathbf{r}, \mathbf{X}) = -u(\mathbf{r}, \mathbf{X})$ for any $\mathbf{X} \in \mathbb{R}^d$ by the antisymmetry of Ψ , and

$$\nabla_{\mathbf{r}} u = \frac{1}{2}(\nabla_j - \nabla_k)\Psi.$$

Then, by the 1-to-1 change of variables on \mathbb{R}^{2d} , with $d\mathbf{x}_j d\mathbf{x}_k = d\mathbf{r} d\mathbf{X}$, and Lemma 5.2,

$$\begin{aligned} \int_{\mathbb{R}^{d(N-2)}} \int_{\mathbb{R}^d \times \mathbb{R}^d} |(\nabla_j - \nabla_k)\Psi|^2 d\mathbf{x}_j d\mathbf{x}_k d\mathbf{x}' &= 4 \int_{\mathbb{R}^{d(N-2)}} \int_{\mathbb{R}^d \times \mathbb{R}^d} |\nabla_{\mathbf{r}} u|^2 d\mathbf{r} d\mathbf{X} d\mathbf{x}' \\ &\geq d^2 \int_{\mathbb{R}^{d(N-2)}} \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{|u|^2}{|\mathbf{r}|^2} d\mathbf{r} d\mathbf{X} d\mathbf{x}' = d^2 \int_{\mathbb{R}^{d(N-2)}} \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{|\Psi|^2}{|\mathbf{x}_j - \mathbf{x}_k|^2} d\mathbf{x}_j d\mathbf{x}_k d\mathbf{x}', \end{aligned}$$

which proves the theorem. \square

The above theorem shows that fermionic particles always feel an inverse-square pairwise repulsion, which is not just due to the energy cost of localization as encoded in the usual uncertainty principle, but which is *strictly stronger* (and in two dimensions therefore non-trivial in contrast to the standard Hardy inequality). Its origin is the relative antipodal antisymmetry and thereby the Poincaré inequality (5.8) which comes weighted by the inverse-square of the distance $r_{jk} = |\mathbf{r}_{jk}|$ between each pair of particles. The repulsion persists also *locally*, i.e. in tubular domains around the diagonals Δ of the configuration space, and independently of the considered boundary conditions. Indeed, an alternative version of

(5.9), without having applied the \mathbb{R}^d -global Hardy inequality in (5.6) but instead the local (diamagnetic) inequality $|\partial_r \Psi| \geq |\partial_r |\Psi||$, and (5.8), is

$$\int_{\mathbb{R}^{dN}} \sum_{j=1}^N |\nabla_j \Psi|^2 dx \geq \frac{4}{N} \int_{\mathbb{R}^{dN}} \sum_{1 \leq j < k \leq N} \left(|\partial_{r_{jk}} |\Psi||^2 + (d-1) \frac{|\Psi(x)|^2}{|\mathbf{x}_j - \mathbf{x}_k|^2} \right) dx \quad (5.10)$$

$$+ \frac{1}{N} \int_{\mathbb{R}^{dN}} \left| \sum_{j=1}^N \nabla_j \Psi \right|^2 dx.$$

Although the first integral of the r.h.s. involves the *bosonic* function $|\Psi| \in L^2_{\text{sym}}(\mathbb{R}^{dN})$, the singular repulsive term forces the probability amplitude $|\Psi|^2$ to be smaller (and even to vanish for $d = 2$) where particles meet, and we will therefore refer to this effect as a **statistical repulsion**⁽¹⁸⁾. One may note however that the constant in (5.9) resp. (5.10) and the number of terms in the sum combine to yield an overall *linear* growth in N , which matches the number of terms of the kinetic energy, but differs from the case of a usual pair interaction of fixed strength, such as in (3.37). Also, the last integral term in (5.9) resp. (5.10) involves the total center-of-mass motion and will typically only contribute to a lower order and may thus often be discarded in applications.

Local, but necessarily more complicated, versions of these inequalities were given for $d = 2$ in [LS13a, LL18]. These may be applied to eventually yield the same type of exclusion bounds as (5.4) and (5.5), with a slightly weaker constant, but with the advantage of opening up for generalizations of the statistical repulsion such as to anyons as discussed in Section 5.6 below. Also note that for dimension $d = 1$ where $H^1_{\text{asym}}(\mathbb{R}^N) \subseteq H^1_0(\mathbb{R}^N \setminus \Delta)$ we actually have a much better inequality from before, namely the many-body Hardy inequality of Theorem 4.11, for which the overall dependence of the r.h.s. is rather *quadratic* in N . Furthermore, in the one-dimensional case with bosons, a vanishing condition on the diagonals Δ is actually sufficient to impose the usual Pauli principle, since there is an equivalence between symmetric functions in $H^1_0(\mathbb{R}^N \setminus \Delta)$ and antisymmetric functions in $H^1(\mathbb{R}^N)$ [Gir60], however this is not the case in $d \geq 2$.

Exercise 5.5. *Prove the radial Hardy inequality (5.7) in two ways: by reducing the usual Hardy inequality to radial functions, and, by modifying the GSR approach of Proposition 4.7.*

5.1.3. *Fermions and determinantal point processes.* Lambert's bonus material...

5.2. **Weaker exclusion.** In the case that one would need to weaken the Pauli principle a bit to allow for, say, up to q particles occupying each one-body state, this could be modeled using a modified N -particle Hilbert space. Let us take

$$\mathcal{H}_{\text{asym}(q)} := \bigotimes^q \left(\bigwedge^K \mathfrak{H} \right), \quad N = qK,$$

which may be thought of as having q different (distinguishable) **flavors** (or **species**) of fermions, with each such flavor being subject to the Pauli principle. In the context of the non-interacting Hamiltonian $\hat{H} = \sum_{j=1}^N \hat{h}_j$ discussed in the beginning of this chapter, the

⁽¹⁸⁾Though, as discussed in [MB03], the term should perhaps be used with some caution.

typical ground state would then be

$$\Psi = (u_0 \wedge \dots \wedge u_{K-1}) \otimes \dots \otimes (u_0 \wedge \dots \wedge u_{K-1})$$

with energy $E_0 = q \sum_{k=0}^{K-1} \lambda_k$. We consider here N to be a multiple of q for simplicity, but this assumption may be relaxed with a slightly more involved framework to specify which flavors are being added. An equivalent and more flexible way to characterize the elements of $\mathcal{H}_{\text{asym}(q)}$ is as functions $\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)$ in $L^2(\mathbb{R}^{dN})$ for which there is a partition of the variables \mathbf{x}_j into q groups, with the variables in each such group being antisymmetric under permutations of the labels.

Because there is also a notion of *spin* in quantum mechanics (recall Exercise 3.7 and Remark 3.28) it is in fact a realistic assumption that each particle comes equipped with such an additional flavor degree of freedom, modeled using an **internal space** \mathbb{C}^q , where $q \geq 1$ is the **spin dimension** of the particle (while the number $s = (d-1)/2 \in \mathbb{Z}_{\geq 0}/2$ is called its **spin**), and the full Hilbert space may then be modeled correctly using $\mathcal{H}_{\text{asym}(q)}$. Although the introduction of spin appears a bit ad hoc here in our context of non-relativistic quantum mechanics, it turns out to be a non-trivial consequence of *relativistic* quantum theory that in nature, i.e. for elementary particles moving in \mathbb{R}^3 , bosons always have q odd (integer spin) while fermions have q even (half-integer spin). In the case of electrons we have $q = 2$, with a basis of \mathbb{C}^2 modeling spin-up respectively spin-down states. The fermions that we have considered previously and modeled by the simpler antisymmetric space $\mathcal{H}_{\text{asym}}$ with $q = 1$ are therefore known as **spinless fermions** and may seem a bit artificial from this perspective, however such particles may become manifest in certain spin-polarized systems.

A simple modification of the proof of Proposition 5.1 to the case $\mathcal{H}_{\text{asym}(q)}$ yields:

Proposition 5.5. *Let $Q \subseteq \mathbb{R}^d$ be a d -cube, $d \geq 1$. For any $N = qK$ with $q, K \geq 1$, and $\Psi \in H^1_{\text{asym}(q)}(Q^N)$, we have*

$$\int_{Q^N} |\nabla \Psi|^2 \geq (N - q)_+ \frac{\pi^2}{|Q|^{2/d}} \int_{Q^N} |\Psi|^2.$$

Again, N being a multiple of q is not important for the proof and may thus be relaxed, as illustrated by the following version (see also [FS12, Lemma 3] for generalizations):

Proposition 5.6. *Let $\Psi \in H^1(\mathbb{R}^{dN})$ be an N -body wave function for which there is a partition of labels into q groups and antisymmetry holds between all variables \mathbf{x}_j in each such group, and let $Q \subseteq \mathbb{R}^d$ be a d -cube, $d \geq 1$. For any subset $A \subseteq \{1, \dots, N\}$ of the particles, $\mathbf{x} = (\mathbf{x}_A; \mathbf{x}_{A^c})$, $n = |A| \geq 0$, and a.e. $\mathbf{x}_{A^c} \in \mathbb{R}^{d(N-n)}$, we have*

$$\int_{Q^n} \sum_{j \in A} |\nabla_j \Psi(\mathbf{x}_A; \mathbf{x}_{A^c})|^2 d\mathbf{x}_A \geq (n - q)_+ \frac{\pi^2}{|Q|^{2/d}} \int_{Q^n} |\Psi(\mathbf{x}_A; \mathbf{x}_{A^c})|^2 d\mathbf{x}_A.$$

Exercise 5.6. *The expression (5.3) approximates the ground-state energy for the **free Fermi gas** (spinless, non-interacting and homogeneous) on a box Q , i.e. the infimum*

$$E_{0, \text{asym}}(N) := \inf \{T[\Psi] : \Psi \in H^1_{\text{asym}}(Q^N), \|\Psi\|_2 = 1\} \approx K_d^{\text{cl}} \rho^{2/d} N,$$

where $\rho = N/|Q|$ is the density. Obtain the approximation for the g.s. energy for the Fermi gas with a fixed number q species of fermions (or q -dimensional spin)

$$E_{0,\text{asym}(q)}(N) := \inf \left\{ T[\Psi] : \Psi \in H_{\text{asym}(q)}^1(Q^N), \|\Psi\|_2 = 1 \right\} \approx q^{-2/d} K_d^{\text{cl}} \rho^{2/d} N. \quad (5.11)$$

Show also that boundary conditions (Dirichlet/Neumann/periodic) on ∂Q are unimportant for the leading-order approximation of the energy.

5.3. Local exclusion and density formulations. We may define the **local n -particle kinetic energy** on a cube Q for fermions, i.e. particles obeying the Pauli principle,

$$e_n(Q; \text{asym}) := \inf_{\substack{\psi \in H_{\text{asym}}^1(Q^n) \\ \int_{Q^n} |\psi|^2 = 1}} \int_{Q^n} \sum_{j=1}^n |\nabla_j \psi|^2,$$

and in general, allowing for q particles to occupy the same state and taking an arbitrary subset n of N total particles on \mathbb{R}^d , those n being localized on Q and the remaining $N - n$ residing anywhere on Q^c ,

$$e_n(Q; \text{asym}(q)) := \inf_{\substack{\Psi \in H_{\text{asym}(q)}^1(\mathbb{R}^{dN}) \\ \Psi|_{Q^n \times (Q^c)^{N-n}} \neq 0}} \text{ess inf}_{\substack{x' \in (Q^c)^{N-n} \\ \Psi|_{Q^n \times \{x'\}} \neq 0}} \frac{\int_{Q^n} \sum_{j=1}^n |\nabla_j \Psi(\cdot; x')|^2}{\int_{Q^n} |\Psi(\cdot; x')|^2}.$$

We found from Proposition 5.1 respectively 5.6 that for these energies

$$e_n(Q; \text{asym}(q)) \geq \frac{\pi^2}{|Q|^{2/d}} (n - q)_+. \quad (5.12)$$

Also note that by translation and permutation symmetries, the above energies are independent of which cube and which subset of particles are considered, thus depending only on the volume (length scale) $|Q|$ and n .

Now, consider an N -body wave function of particles on \mathbb{R}^d , $\Psi \in H_{\text{asym}(q)}^1(\mathbb{R}^{dN})$, and a partition \mathcal{P} of the configuration space into d -cubes Q with a corresponding kinetic energy

$$\langle \Psi, \hat{T} \Psi \rangle = T[\Psi] = \sum_{Q \in \mathcal{P}} T^Q[\Psi],$$

where we recall the local expected kinetic energy on the domain Q (see Section 4.8)

$$T^Q[\Psi] := \sum_{j=1}^N \int_{\mathbb{R}^{dN}} |\nabla_j \Psi|^2 \mathbf{1}_Q(\mathbf{x}_j) dx. \quad (5.13)$$

Lemma 5.7 (Local exclusion principle). *For any d -cube Q and L^2 -normalized N -body state $\Psi \in H_{\text{asym}(q)}^1(\mathbb{R}^{dN})$ we have*

$$T^Q[\Psi] \geq \frac{\pi^2}{|Q|^{2/d}} \left(\int_Q \varrho_\Psi(\mathbf{x}) dx - q \right)_+. \quad (5.14)$$

Proof. We insert the partition of unity (3.44) into the definition (5.13), producing

$$\begin{aligned} T^Q[\Psi] &= \sum_{A \subseteq \{1, \dots, N\}} \int_{(Q^c)^{N-|A|}} \int_{Q^{|A|}} \sum_{j \in A} |\nabla_j \Psi|^2 \prod_{k \in A} d\mathbf{x}_k \prod_{k \notin A} d\mathbf{x}_k \\ &\geq \sum_{A \subseteq \{1, \dots, N\}} \int_{(Q^c)^{N-|A|}} e_{|A|}(Q; \text{asym}(q)) \int_{Q^{|A|}} |\Psi|^2 \prod_{k \in A} d\mathbf{x}_k \prod_{k \notin A} d\mathbf{x}_k \\ &= \sum_{n=0}^N e_n(Q; \text{asym}(q)) p_{n,Q}[\Psi], \end{aligned}$$

that is the least possible energy weighted over the particle distribution induced from Ψ . Now, we simply apply the bound (5.12) and use convexity of the function $x \mapsto (x - q)_+$,

$$T^Q[\Psi] \geq \sum_{n=0}^N \frac{\pi^2}{|Q|^{2/d}} (n - q)_+ p_{n,Q}[\Psi] \geq \frac{\pi^2}{|Q|^{2/d}} \left(\sum_{n=0}^N n p_{n,Q}[\Psi] - q \right)_+,$$

which by (3.43) is exactly the r.h.s. of (5.14). \square

Example 5.8 (The free Fermi gas). As a simple application of this local bound we may prove a global lower bound for the ground-state energy of the ideal Fermi gas which matches the approximation (5.11) apart from the explicit value of the constant, i.e. proving that the fermionic energy indeed is extensive in the number of particles, with only the simple bound (5.12) as input. Namely, consider an arbitrary wave function of N fermions confined to a large cube $Q_0 = [0, L]^d$,

$$\Psi \in H_{\text{asym}(q)}^1(Q_0^N) \quad \Rightarrow \quad \varrho_\Psi \in L^1(Q_0; \mathbb{R}_+).$$

Taking a partition \mathcal{P} of Q_0 into exactly M^d smaller cubes $Q \in \mathcal{P}$, of equal size $|Q| = |Q_0|/M^d$, $M \in \mathbb{N}$, the energy is by Lemma 5.7 bounded as

$$\begin{aligned} T[\Psi] &= \sum_{Q \in \mathcal{P}} T^Q[\Psi] \geq \sum_{Q \in \mathcal{P}} \frac{\pi^2}{|Q|^{2/d}} \left(\int_Q \varrho_\Psi(\mathbf{x}) d\mathbf{x} - q \right) = \frac{\pi^2}{|Q|^{2/d}} \left(\int_{Q_0} \varrho_\Psi(\mathbf{x}) d\mathbf{x} - qM^d \right) \\ &= \frac{\pi^2}{|Q_0|^{2/d}} \left(NM^2 - qM^{d+2} \right). \end{aligned}$$

Optimizing this expression in M gives $M \sim \left(\frac{2N}{(d+2)q} \right)^{1/d}$ (rounded to the nearest integer) and thus

$$E_{0, \text{asym}(q)}(N) := \inf_{\substack{\Psi \in L^2_{\text{asym}(q)}(Q_0^N) \\ \|\Psi\|=1}} T[\Psi] \geq \frac{d}{d+2} \left(\frac{2}{d+2} \right)^{2/d} \frac{\pi^2}{q^{2/d}} \frac{N^{1+2/d}}{|Q_0|^{2/d}} + \frac{O(N^{1+1/d})}{|Q_0|^{2/d}}.$$

Hence, with q fixed and taking both $N \rightarrow \infty$ and $|Q_0| \rightarrow \infty$ at fixed density $\rho := N/|Q_0|$, what may commonly be referred to as the **thermodynamic limit**, the energy per particle

is⁽¹⁹⁾

$$\liminf_{\substack{N, |Q_0| \rightarrow \infty \\ \rho = N/|Q_0|}} \frac{E_{0, \text{asym}(q)}(N)}{N} \geq \frac{d}{d+2} \left(\frac{2}{d+2} \right)^{2/d} \pi^2 \frac{\rho^{2/d}}{q^{2/d}},$$

to be compared with (5.11) and (5.3). Note that when $q = N$, i.e. for bosons, M cannot be chosen large and in fact the local bound (5.14) is trivial for any Q . This reflects the fact that the energy for the ideal Bose gas on Q_0 is $E_{0, \text{sym}}(N) = N\lambda_0(-\Delta_{Q_0})$ which is linear in N and also depends crucially on the boundary conditions chosen on ∂Q_0 . In the thermodynamic limit one obtains in any case $E_{0, \text{sym}}(N)/N \rightarrow 0$ for noninteracting bosons.

Exercise 5.7. Compute the n -particle probability distribution $p_{n, Q}[\Psi_0]$ for the bosonic Neumann ground state Ψ_0 on Q_0^N in terms of $t = |Q|/|Q_0|$. What can be said about the corresponding problem for the fermionic ground state (difficult, but perhaps with a change of geometry and selection of states)?

5.4. Repulsive bosons. We will now use a formal analogy and treat a repulsive interaction between bosons or distinguishable particles as a form of exclusion principle. Indeed the effect of such an interaction will typically be to reduce the probability density $|\Psi(\mathbf{x})|^2$ around the 2-particle diagonals Δ , and strong enough interactions could even enforce a vanishing condition

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = 0 \quad \text{if } \mathbf{x}_j = \mathbf{x}_k \text{ for some } j \neq k, \quad (5.15)$$

thereby embodying a weak Pauli-type exclusion principle on the configuration space $\mathcal{C}^{d \times N}$ or $\mathcal{C}_{\text{sym}}^{d \times N}$. Another motivation for considering this type of generalization comes from the fermionic Hardy inequality in Theorem 5.4, which shows that effects of the exchange statistics of the particles may actually be estimated concretely by some sort of repulsive interaction. This approach also turns out to be useful for anyons which can be treated as bosons with magnetic repulsive interactions.

5.4.1. Pairwise interactions. In the case that there is a given pair-interaction potential W between particles, we define the corresponding n -particle energy on the box Q ,

$$e_n(Q; W) := \inf_{\int_{Q^n} |\psi|^2 = 1} \int_{Q^n} \left(\sum_{j=1}^n |\nabla_j \psi|^2 + \sum_{1 \leq j < k \leq n} W(\mathbf{x}_j - \mathbf{x}_k) |\psi|^2 \right) dx.$$

Note that e_n with $n \geq 2$ can be reduced to a bound in terms of only e_2 , namely:

Lemma 5.9. For any pair-interaction potential W and any d -cube Q , and $n \geq 2$, we have

$$e_n(Q; W) \geq \frac{n}{2} e_2(Q; (n-1)W).$$

Proof. Use the simple identity

$$(n-1) \sum_{j=1}^n |\nabla_j \psi|^2 = \sum_{1 \leq j < k \leq n} (|\nabla_j \psi|^2 + |\nabla_k \psi|^2)$$

⁽¹⁹⁾Here we take the lim inf for generality, though the limit actually exists by the Weyl asymptotic formula (cf. Exercise 5.2).

to bound the n -body energy in terms of a sum of two-body energies:

$$e_n(Q; W) = \inf_{\int_{Q^n} |\psi|^2 = 1} \frac{1}{n-1} \sum_{j < k} \int_{Q^n} (|\nabla_j \psi|^2 + |\nabla_k \psi|^2 + (n-1)W(\mathbf{x}_j - \mathbf{x}_k)|\psi|^2) dx,$$

where each term of the sum is bounded below by $e_2(Q; (n-1)W) \int_{Q^n} |\psi|^2$. \square

This tells us that, as soon as the two-particle energy is strictly positive, such as for repulsive pair interactions, there will be positive energy also for $n \geq 2$ particles, analogously to the Pauli principle. We also note that for any n and non-negative pair potential W the function $f(\mu) := e_n(Q; \mu W)$ is monotone increasing and concave in $\mu \geq 0$ (an infimum of affine functions), and $f(0) = 0$.

Let us consider some examples.

5.4.2. The stupid bound. In the case that $W(\mathbf{x}) = W_\beta(\mathbf{x}) := \beta|\mathbf{x}|^{-2}$, $\beta \geq 0$, that is an inverse-square repulsion, we may use the following very crude bound for e_n :

$$e_n(Q; W_\beta) \geq \sum_{j < k} \inf_{\int_{Q^n} |\psi|^2 = 1} \int_{Q^n} W_\beta(\mathbf{x}_j - \mathbf{x}_k) |\psi|^2 \geq \binom{n}{2} \inf_{\mathbf{x}_1, \mathbf{x}_2 \in Q} W_\beta(\mathbf{x}_1 - \mathbf{x}_2) \geq \frac{\beta n(n-1)}{2d|Q|^{2/d}}$$

(in fact we don't even need the kinetic energy in this case). In particular,

$$e_n(Q; W_\beta) \geq \frac{\beta}{d|Q|^{2/d}} (n-1)_+. \quad (5.16)$$

5.4.3. Hard-core bosons. For the case of a hard-sphere interaction W_R^{hs} in $d = 3$ (see Example 3.20), one can derive the rough bound [LPS15, Proposition 10]

$$e_2(Q; W_R^{\text{hs}}) \geq \frac{2}{\sqrt{3}} \frac{R}{|Q|} (2 - R/|Q|^{1/3})_+^{-2}.$$

Note that it vanishes as $R \rightarrow 0$ (the dilute limit; cf. Exercise 5.8).

5.4.4. The Lieb–Liniger model. In one dimension, the value of a function at a point may be controlled by the kinetic energy and the overall normalization (recall (4.15)), and thus it is possible to define a point interaction of the type $W_{\text{LL}}(x) = \delta(x)$ in the form sense, that is

$$e_n(Q; \eta W_{\text{LL}}) = \inf_{\int_{Q^n} |\psi|^2 = 1} \int_{Q^n} \left(\sum_{j=1}^n \left| \frac{\partial \psi}{\partial x_j} \right|^2 + \eta \sum_{1 \leq j < k \leq n} \delta(x_j - x_k) |\psi|^2 \right) dx.$$

This is also known as the **Lieb–Liniger model** [LL63], and for any $\eta \geq 0$ one has (exercise)

$$e_2(Q; \eta W_{\text{LL}}) = 4\xi_{\text{LL}}(\eta|Q|/4)^2/|Q|^2, \quad (5.17)$$

where $\xi_{\text{LL}}(x)$ is defined as the smallest root $\xi \geq 0$ of $\xi \tan \xi = x$,

$$\xi_{\text{LL}}(x) \approx \arctan \sqrt{x + 4x^2/\pi^2} \sim \begin{cases} \sqrt{x}, & x \rightarrow 0^+, \\ \pi/2, & x \rightarrow \infty. \end{cases}$$

Note that this model interpolates continuously between non-interacting bosons with $e_2 = 0$ for $\eta = 0$ and hard-core bosons (or fermions; cf. remarks in Section 5.1.2) with $e_2 = \pi^2/|Q|^2$ for $\eta = +\infty$. Indeed it has been considered as a model for **intermediate statistics** in one dimension; see e.g. [LM77, Myr99, LS13b, LS14].

5.4.5. *Local exclusion for pairwise interacting bosons.* Define the corresponding **expected interaction energy** on Q ,

$$W^Q[\Psi] := \frac{1}{2} \sum_{j=1}^N \sum_{(j \neq) k=1}^N \int_{\mathbb{R}^{dN}} W(\mathbf{x}_j - \mathbf{x}_k) |\Psi|^2 \mathbf{1}_Q(\mathbf{x}_j) d\mathbf{x},$$

as well as the combined energies

$$(T + W)^Q[\Psi] := T^Q[\Psi] + W^Q[\Psi].$$

Then, for a partition \mathcal{P} of \mathbb{R}^d ,

$$T[\Psi] + W[\Psi] = \sum_{Q \in \mathcal{P}} (T + W)^Q[\Psi].$$

Lemma 5.10 (Local exclusion principle for pairwise repulsion). *Let $W \geq 0$ be a repulsive pair interaction. For any d -cube Q and N -body wave function $\Psi \in H^1(\mathbb{R}^{dN})$ we have*

$$(T + W)^Q[\Psi] \geq \frac{1}{2} e_2(Q; W) \left(\int_Q \varrho_\Psi(\mathbf{x}) d\mathbf{x} - 1 \right)_+.$$

Proof. The proof is a straightforward extension of the proof of Lemma 5.7 where we use Lemma 5.9, monotonicity $e_2(Q; (n-1)W) \geq e_2(Q; W)$, and that $|A|/2 \geq (|A| - 1)_+/2$ for $|A| \geq 2$. Non-negativity of W is used in order to estimate the interactions between particles inside and outside Q trivially,

$$\begin{aligned} T^Q[\Psi] &= \frac{1}{2} \sum_{A \subseteq \{1, \dots, N\}} \sum_{j \in A} \sum_{\substack{k=1 \\ k \neq j}}^N \int_{\mathbb{R}^{dN}} W(\mathbf{x}_j - \mathbf{x}_k) |\Psi(\mathbf{x})|^2 \mathbf{1}_{\mathbf{x}_j \in A} \mathbf{1}_{\mathbf{x}_k \notin A} d\mathbf{x} \\ &\geq \frac{1}{2} \sum_{A \subseteq \{1, \dots, N\}} \sum_{\substack{j, k \in A \\ j \neq k}} \int_{\mathbb{R}^{dN}} W(\mathbf{x}_j - \mathbf{x}_k) |\Psi(\mathbf{x})|^2 \mathbf{1}_{\mathbf{x}_j \in A} \mathbf{1}_{\mathbf{x}_k \in A} d\mathbf{x}, \end{aligned}$$

which is only a significant loss if the support of W is relatively large. \square

Application: just as a local application of Lemma 5.7 gave rise to bounds for the homogeneous Fermi gas as in Example 5.8, Lemma 5.10 can be used to prove lower bounds for homogeneous interacting Bose gases; see [LPS15] for examples.

Exercise 5.8. *Consider the strength of the hard-core repulsion as the size of the core goes to zero, in different dimensions $d = 1, 2, 3$. For simplicity, pass to the relative coordinate \mathbf{r} only and consider the g.s. energy on $B_1(0)$ with a vanishing condition on $B_\varepsilon(0)$, $0 < \varepsilon < 1$. Note that for $d = 1$ it stays bounded in the limit $\varepsilon \rightarrow 0$ while for $d \geq 2$ it vanishes, reflecting Lemma 4.8. (Hint: consider trial states of the form $u(r) = (r - \varepsilon)_+$ resp. $u(r) = \ln_+(r/\varepsilon)$ and constant for some $r > a > \varepsilon$.)*

Exercise 5.9. *Prove (5.17) by considering the function on $Q^2 = [0, L]^2$*

$$\psi(x_1, x_2) = \cos \left[2\xi_{\text{LL}}(\eta L/4) \left(\frac{X}{L} - \frac{1}{2} \right) \right] \cos \left[\xi_{\text{LL}}(\eta L/4) \left(\frac{|x|}{L} - 1 \right) \right]$$

in the relative coordinates $X = (x_1 + x_2)/2 \in [0, L]$, $x = x_1 - x_2$. Note that it is positive, symmetric and satisfies the corresponding boundary conditions

$$\partial_x \psi|_{x=0^+} = \frac{\eta}{4} \psi|_{x=0^+}, \quad \partial_{x_1} \psi|_{x_1=0} = \left(\frac{1}{2} \partial_X + \partial_x \right) \psi|_{X+\frac{x}{2}=0} = 0, \quad \text{etc.}$$

5.5. Scale-covariant systems. In the case of still weaker notions of exclusion, such as only the vanishing condition (5.15) (whenever it can be formalized as a nontrivial condition; cf. Exercise 5.8), we cannot simply rely on the number of terms of the interaction as above to yield a sufficient bound. The following lemma (introduced in [LLN19] as a refinement of a strategy in [LS18]) shows that if the corresponding energy e_n satisfies a scale-covariance property, such as $e_n(\lambda Q; W_\beta) = \lambda^{-2} e_n(Q; W_\beta)$, $\lambda > 0$, for inverse-square repulsion, and eventually becomes strictly positive with n large enough (thus accommodating interactions not only between pairs of particles), then it will necessarily grow *superlinearly* with n .

Lemma 5.11 (Covariant energy bound; [LLN19, Lemma 4.1]). *Assume that to any $n \in \mathbb{N}_0$ and any cube $Q \subset \mathbb{R}^d$ there is associated a non-negative number ('energy') $e_n(Q)$ satisfying the following properties, for some constant $s > 0$:*

- (scale-covariance) $e_n(\lambda Q) = \lambda^{-2s} e_n(Q)$ for all $\lambda > 0$;
- (translation-invariance) $e_n(Q + \mathbf{x}) = e_n(Q)$ for all $\mathbf{x} \in \mathbb{R}^d$;
- (superadditivity) For any collection of disjoint cubes $\{Q_j\}_{j=1}^J$ such that their union is a cube,

$$e_n\left(\bigcup_{j=1}^J Q_j\right) \geq \min_{\{n_j\} \in \mathbb{N}_0^J \text{ s.t. } \sum_j n_j = n} \sum_{j=1}^J e_{n_j}(Q_j);$$

- (a priori positivity) There exists $q \geq 0$ such that $e_n(Q) > 0$ for all $n \geq q$.

Then there exists a constant $C > 0$ independent of n and Q such that

$$e_n(Q) \geq C |Q|^{-2s/d} n^{1+2s/d}, \quad \forall n \geq q. \quad (5.18)$$

Proof. Note that for $q \leq n \leq N$, (5.18) holds for some $C = C_N > 0$ by the a priori positivity. What we aim to do is to remove the N -dependence of this constant.

Denote $E_n := e_n(Q_0)$ with $Q_0 = [0, 1]^d$. Assume by induction in N that

$$E_n \geq C n^{1+2s/d}, \quad \forall q \leq n \leq N - 1 \quad (5.19)$$

with a uniform constant $C > 0$ and consider $n = N$. Split Q_0 into 2^d subcubes of half side length and obtain by the superadditivity, translation-invariance and scale-covariance

$$E_N \geq 2^{2s} \min_{\{n_j\} \text{ s.t. } \sum_j n_j = N} \sum_{j=1}^{2^d} E_{n_j}. \quad (5.20)$$

Consider a configuration $\{n_j\} \subset \mathbb{N}_0^{2^d}$ such that the minimum in (5.20) is attained. The a priori positivity $E_N > 0$ ensures that none of the n_j can be N (in the same way we deduce that $E_0 = 0$). Assume that there exist exactly M numbers $n_j < q$ with $0 \leq M \leq 2^d$. Then

$$\sum_{n_j \geq q} 1 = 2^d - M \quad \text{and} \quad \sum_{n_j \geq q} n_j = N - \sum_{n_j < q} n_j \geq N - qM.$$

Therefore, from (5.20), (5.19) and Hölder's inequality we deduce that

$$E_N \geq C2^{2s} \sum_{n_j \geq q} n_j^{1+2s/d} \geq C2^{2s} \frac{\left(\sum_{n_j \geq q} n_j\right)^{1+2s/d}}{\left(\sum_{n_j \geq q} 1\right)^{2s/d}} \geq CN^{1+2s/d} \frac{(1 - qMN^{-1})^{1+2s/d}}{(1 - M2^{-d})^{2s/d}} \quad (5.21)$$

with the same constant C as in (5.19). If we take

$$N \geq q2^d \left(1 + \frac{d}{2s}\right),$$

so that also $qMN^{-1} \leq 1$, then by Bernoulli's inequality

$$(1 - qMN^{-1})^{1+d/(2s)} \geq 1 - qMN^{-1} \left(1 + \frac{d}{2s}\right) \geq 1 - M2^{-d},$$

and hence (5.21) reduces to

$$E_N \geq CN^{1+2s/d} \quad (5.22)$$

with the same constant C as in (5.19).

By induction we obtain (5.22) for all $N \geq q$, with a constant C independent of N . This is the desired bound (5.18) for the unit cube Q_0 . The result for the general cube follows from scale-covariance and translation-invariance. \square

With a superlinear growth in the energy by the number of particles we may obtain local exclusion principles of the previous form. The following is a version of [LLN19, Lemma 4.4].

Lemma 5.12 (Local exclusion principle for scale-covariant systems). *Assume that to each $n \in \mathbb{N}_0$ we have an n -body energy operator \hat{T}_n resp. form $T_n[\Psi] = \langle \Psi, \hat{T}_n \Psi \rangle = \sum_{j=1}^n T_{n,j}[\Psi]$ on $L^2(\mathbb{R}^{dn})$ which restricts to a local operator $\hat{T}_n|_{Q^n}$ resp. form on $L^2(Q^n)$ such that its corresponding local n -particle energies*

$$e_n(Q) := \inf_{\psi \in \mathcal{Q}(\hat{T}_n|_{Q^n}) \setminus \{0\}} \langle \hat{T}_n|_{Q^n} \psi, \psi \rangle = \inf_{\psi \in \mathcal{Q}(\hat{T}_n|_{Q^n}) \setminus \{0\}} \frac{\sum_{j=1}^n T_{n,j}[\psi]}{\|\psi\|^2}$$

satisfy the assumptions of Lemma 5.11. Furthermore, assume that for any d -cube Q and L^2 -normalized N -body wave function $\Psi \in \mathcal{Q}(\hat{T}_N)$ the expected energy on Q ,

$$T_N^Q[\Psi] := \sum_{j=1}^N T_{N,j}[\Psi \mathbf{1}_{\mathbf{x}_j \in Q}],$$

admits a decomposition or lower bound of the form

$$T_N^Q[\Psi] \geq \sum_{A \subseteq \{1, \dots, N\}} \int_{(Q^c)^{N-|A|}} \langle \Psi(\cdot; \mathbf{x}_{A^c}), \hat{T}_{|A|}|_{Q^{|A|}} \Psi(\cdot; \mathbf{x}_{A^c}) \rangle_{L^2(Q^{|A|})} d\mathbf{x}_{A^c}. \quad (5.23)$$

Then

$$T_N^Q[\Psi] \geq Cq^{2s/d} |Q|^{-2s/d} \left(\int_Q \varrho_\Psi(\mathbf{x}) d\mathbf{x} - q \right)_+,$$

with the same constant C as in (5.18).

Proof. The proof follows exactly as the proof of Lemma 5.7: by (5.23),

$$T_N^Q[\Psi] \geq \sum_{n=0}^N e_n(Q) p_{n,Q}[\Psi],$$

where, by Lemma 5.11,

$$e_n(Q) \geq C|Q|^{-2s/d} n^{1+2s/d} \mathbf{1}_{n \geq q} \geq C|Q|^{-2s/d} q^{2s/d} [n - q]_+$$

for all $n \geq 0$. \square

Superadditivity for the usual kinetic energy with $s = 1$, and also its fractional version with arbitrary $s > 0$, essentially follows immediately from the form decomposition

$$(-\Delta)|_Q^s \geq \sum_{j=1}^J (-\Delta)|_{Q_j}^s, \quad Q = \cup_{j=1}^J Q_j,$$

where in the purely fractional (non-local) case $s \notin \mathbb{N}$ there may be some loss in the interaction between different cubes. Compare to the proof of Lemma 5.10, and see [LLN19, Lemma 4.3] for details.

Exercise 5.10. *It is in Lemma 5.11 possible to allow for $E_n < 0$ for finitely many $n > 0$ under a small refinement of the assumption concerning a priori positivity. Show that it is sufficient that there exists $q > 0$ and $c > 1$ such that for all $n \geq q$*

$$E_n > c \frac{d}{2s} 2^{d+2s} E_-, \quad E_- := \max_{0 \leq n < q} (-E_n).$$

Namely, with this assumption, the bound in (5.21) may again be used for all $n_j \geq q$, and one obtains $E_N \geq CN^{1+2s/d} f(M/2^d)$, $C = \min_{q \leq n \leq N-1} E_n/n^{1+2s/d}$, where the function

$$f(x) := \frac{(1 - q2^d N^{-1}x)^{1+2s/d}}{(1-x)^{2s/d}} - \frac{E_- 2^{d+2s}}{CN^{1+2s/d}} x, \quad x \in [0, 1),$$

is strictly increasing if N is large enough.

5.6. Anyons. We end this chapter with a short discussion on the exclusion properties of anyons in two dimensions (recall their definition in Section 3.7). Two-particle energies and other pairwise statistics-dependent properties for anyons have been known since the original works [LM77, Wil82, ASWZ85] in the abelian case, and at least since [Ver91, LO94] for certain non-abelian anyons, however the method outlined below to account for statistical repulsion in the full many-body context is fairly recent and developed in [LS13a, LS13b, LS14, LL18, Lun17, Qva17, LS18].

For (ideal abelian) anyons one has the following many-body Hardy inequality, which was generalized from the fermionic one (5.10) in [LS13a, Theorem 4] and [LL18, Theorem 1.3]:

Theorem 5.13 (Many-anyon Hardy). *For any $\alpha \in \mathbb{R}$, $N \geq 1$, and $\Psi \in \mathcal{Q}(\hat{T}_\alpha)$, one has the many-body Hardy inequality*

$$\langle \Psi, \hat{T}_\alpha \Psi \rangle \geq \frac{4}{N} \int_{\mathbb{R}^{dN}} \sum_{1 \leq j < k \leq N} \left(|\partial_{r_{jk}} \Psi|^2 + \alpha_N^2 \frac{|\Psi(\mathbf{x})|^2}{r_{jk}^2} \right) dx + \frac{1}{N} \int_{\mathbb{R}^{dN}} \left| \sum_{j=1}^N \nabla_j \Psi \right|^2 dx, \quad (5.24)$$

where $r_{jk} = |\mathbf{x}_j - \mathbf{x}_k|$, and the strength of the statistical repulsion term depends on the anyonic statistics parameter α via

$$\alpha_N := \min_{p \in \{0, 1, \dots, N-2\}} \min_{q \in \mathbb{Z}} |(2p+1)\alpha - 2q|. \quad (5.25)$$

The expression (5.25) is a piecewise linear and 2-periodic function of α (in accordance with the periodicity of the exchange phase) and for $N = 2$ it reduces to the simple form of a saw-tooth wave with $\alpha_2 = |\alpha|$ for $\alpha \in [-1, 1]$, having maxima at $\alpha \in 2\mathbb{Z} + 1$ (fermions) and minima at $\alpha \in 2\mathbb{Z}$ (bosons). However, in the limit as $N \rightarrow \infty$ the expression depends non-trivially on arithmetic properties of α (see [LS13a, Proposition 5]):

$$\alpha_* := \lim_{N \rightarrow \infty} \alpha_N = \inf_{N \geq 2} \alpha_N = \begin{cases} \frac{1}{\nu}, & \text{if } \alpha = \frac{\mu}{\nu} \in \mathbb{Q} \text{ reduced, } \mu \text{ odd and } \nu \geq 1, \\ 0, & \text{otherwise.} \end{cases}$$

In other words, it is supported only on the rationals with odd numerator, with a magnitude inversely proportional to the denominator, and may thus be considered a variant of a function known as the **Thomae**, or **popcorn function**.

*Remark** 5.14. In order to understand the origin of the above expressions and their peculiar dependence on α , recall that anyons may be modeled rigorously using connections on fiber bundles; cf. (3.53) and Remark 3.29. The kinetic energy for N anyons may in fact be written as

$$\hat{T}_\alpha = \sum_{j=1}^N (-i\nabla_{\mathbf{x}_j}^{\mathbf{A}_\alpha})^2,$$

where \mathbf{A}_α denotes a connection one-form (gauge potential) on the bundle which implements the statistics, i.e. which is such that the holonomies produced under continuous exchanges of the particles yield the corresponding representation of the braid group, $\rho: B_N \rightarrow \mathbf{U}(\mathcal{F})$, of the anyon model. For abelian anyons, with fiber $\mathcal{F} = \mathbb{C}$ and statistics parameter $\alpha \in [0, 2)$, this is thus the phase $\rho(\tau_{n_1} \dots \tau_{n_k}) = e^{i\alpha\pi k}$ of the exchange as discussed in Exercises 3.13-3.14.

The Poincaré inequality (5.8) that was used for the statistical repulsion of fermions is here replaced by the inequality

$$\int_{r\mathbb{S}^1} |\nabla_{\mathbf{r}}^{\mathbf{A}_\alpha} \Psi|^2 \geq \int_{r\mathbb{S}^1} \left(|\partial_r |\Psi||^2 + \min_{q \in \mathbb{Z}} |\Phi(r) - 2q|^2 \frac{1}{r^2} |\Psi|^2 \right), \quad (5.26)$$

where the integration is performed over the circle $|\mathbf{r}| = r$ in the relative coordinates $\mathbf{r} = \mathbf{r}_{jk}$ of a fixed pair $\mathbf{x}_j, \mathbf{x}_k$ of particles, and $2\pi\Phi(r)$ is defined as the statistics phase (i.e. the holonomy on the bundle) obtained under exchange of this pair as $\mathbf{r} \rightarrow -\mathbf{r} \rightarrow \mathbf{r}$ continuously along the full circle $r\mathbb{S}^1$. Note that already after half of the circle has been traversed one has actually completed a full particle exchange, $\mathbf{r} \rightarrow -\mathbf{r} \sim \mathbf{r}$, and thus the corresponding phase factor in this case must be (see Exercise 3.14)

$$e^{i\pi\Phi(r)}, \quad \Phi(r) = (1 + 2p(r))\alpha,$$

where $p(r) \in \{0, 1, \dots, N-2\}$ denotes the number of other particles that are enclosed under such an exchange. This depends both on the positions of the other $N-2$ particles $\mathbf{x}' = (\mathbf{x}_l)_{l \neq j, k}$, on the center of mass \mathbf{X} of the particle pair, and on the radius r of the circle. However, recall that the phase is only determined uniquely up to multiples of 2π , i.e.

$e^{i\pi\Phi(r)} = e^{i\pi(\Phi(r)-2q)}$ for any $q \in \mathbb{Z}$. Let us for definiteness take the representative closest to the identity,

$$e^{i\pi\beta_0}, \quad \beta_0 = \beta_0(r) := \pm \min_{q \in \mathbb{Z}} |\Phi(r) - 2q|,$$

where one of the signs apply and $\beta_0 \in (-1, 1]$. This phase factor may be considered as a non-trivial boundary condition that the function $u(\varphi) := \Psi(\mathbf{r}(r; \varphi), \mathbf{X}; \mathbf{x}')$ of the relative angle φ (with r , \mathbf{X} and \mathbf{x}' fixed) must satisfy:

$$u(\pi) = e^{i\pi\beta_0} u(0). \quad (5.27)$$

It is a straightforward exercise (see below) to show that the Poincaré inequality

$$\int_0^\pi |u'(\varphi)|^2 d\varphi \geq \beta_0^2 \int_0^\pi |u(\varphi)|^2 d\varphi \quad (5.28)$$

holds for such semi-periodic functions on the (half) circle, by expanding in the basis of energy eigenstates $u_q(\varphi) = e^{i(\beta_0+2q)\varphi}$, $q \in \mathbb{Z}$. Proceeding as in (5.6) one then obtains (5.26), and finally (5.24) after minimizing over all possibilities for $p(r)$, i.e. $\beta_0(r) \geq \alpha_N$ for all r . Note that in the case $\alpha = 0$ one has $\beta_0 \equiv 0$ and thus bosons and no Poincaré inequality, while for $\alpha = 1$ one has $\beta_0 = \min_{q \in \mathbb{Z}} |1 + 2p(r) - 2q| \equiv 1$ and thus the fermionic Poincaré inequality (5.8). The above procedure may even be extended to certain families of non-abelian anyons [Qva17, LQ18].

The following generalization of the diamagnetic inequality (4.27) holds despite the magnetic vector potentials in (3.53) not being locally square integrable around the diagonals:

Lemma 5.15 (Diamagnetic inequality for anyons [LS14, Lemma 4]). *Given any $\alpha \in \mathbb{R}$ and $\Psi \in \mathcal{Q}(\hat{T}_\alpha)$ we have $|\Psi| \in \mathcal{Q}(\hat{T}_0) = H_{\text{sym}}^1$ and $T_\alpha[\Psi] \geq T_0[|\Psi|]$, and in particular the g.s. energy for anyons is always greater than or equal to the corresponding bosonic g.s. energy.*

Let us denote by (which needs to be interpreted in the correct form sense [LS14, LL18])

$$e_n(\alpha) := \inf_{\int_{Q_0^n} |\Psi|^2 = 1} \left\langle \Psi, \hat{T}_\alpha \Psi \right\rangle_{L^2(Q_0^n)}$$

the local (Neumann) n -particle kinetic energy for anyons on the unit square $Q_0 = [0, 1]^2$ (the corresponding energy on a general square $Q \subseteq \mathbb{R}^2$ is obtained by simple scaling due to homogeneity of the kinetic energy). A local version of Theorem 5.13 may be used to prove that e_n satisfies a lower bound for all n of the form [LL18]

$$e_n(\alpha) \geq f((j'_{\alpha_n})^2)(n-1)_+,$$

where j'_ν denotes the first positive zero of the derivative of the Bessel function J_ν of the first kind,

$$\sqrt{2\nu} \leq j'_\nu \leq \sqrt{2\nu(1+\nu)} \quad (\text{and } j'_0 := 0),$$

and $f: [0, (j'_1)^2] \rightarrow \mathbb{R}_+$ is a function satisfying

$$t/6 \leq f(t) \leq 2\pi t \quad \text{and} \quad f(t) = 2\pi t(1 - O(t^{1/3})) \quad \text{as } t \rightarrow 0.$$

Proceeding as in Example 5.8, one may then prove that the ground-state energy per particle and unit density of the ideal anyon gas in the thermodynamic limit at fixed density $\rho = N/|Q|$,

$$e(\alpha) := \liminf_{N \rightarrow \infty, |Q| \rightarrow \infty} \frac{|Q|^{-1} e_N(\alpha)}{N\rho} = \liminf_{N \rightarrow \infty} \frac{e_N(\alpha)}{N^2},$$

is bounded from below by

$$e(\alpha) \geq \frac{1}{24} (j'_{\alpha_*})^2 \geq \frac{1}{12} \alpha_*,$$

and moreover, as $\alpha_* \rightarrow 0$ the bound improves to

$$e(\alpha) \geq \pi \alpha_* (1 - O(\alpha_*^{1/3})).$$

The dependence of the above expressions on α_* comes about by assuming (as a lower bound) that the measure of relative radii $r = |\mathbf{x}_j - \mathbf{x}_k|$ such that the factor $\beta_0(r)^2$ of the potential in (5.26) differs from its absolute minimum α_*^2 can be vanishingly small. This requires the gas to be dilute and its particles arranged in tiny clusters [LL18, Lun17], and it is not clear that such configurations will be beneficial with respect to the uncertainty principle. Indeed, recently [LS18] the above bounds have been improved by using the scale covariance of ideal anyons (cf. Lemma 5.12; for superadditivity see [LS18, Lemma 4.2]) and the uncertainty principle, to yield a dependence only on the two-particle energy:

Lemma 5.16 (Local exclusion principle for anyons [LS18]). *For any $\alpha \in \mathbb{R}$ and $n \geq 2$, it holds*

$$e_n(\alpha) \geq c(\alpha)n,$$

where

$$c(\alpha) := \frac{1}{4} \min\{e_2(\alpha), e_3(\alpha), e_4(\alpha)\} \geq \frac{1}{4} \min\{e_2(\alpha), 0.147\}.$$

Furthermore, for any N -anyon wave function $\Psi \in \mathcal{Q}(\hat{T}_\alpha)$ and any square Q we have the local exclusion principle

$$T_\alpha^Q[\Psi] \geq \frac{c(\alpha)}{|Q|} \left(\int_Q \rho_\Psi(\mathbf{x}) d\mathbf{x} - 1 \right)_+.$$

In fact, these lower bounds in terms of $e_2(\alpha) \geq \frac{1}{3}\alpha_2$ may be complemented with upper bounds of the same form, and one has the following leading behavior for the ground state energy of the ideal anyon gas, showing that it has a similar extensivity as the Fermi gas for all types of anyons except for bosons:

Theorem 5.17 (Extensivity of the ideal anyon gas energy [LS18]). *There exist constants $0 < C_1 \leq C_2 < \infty$ such that for any $\alpha \in \mathbb{R}$*

$$C_1 \alpha_2 \leq e(\alpha) \leq C_2 \alpha_2,$$

and moreover, in the limit $\alpha_2 \rightarrow 0$,

$$e(\alpha) \geq \frac{\pi}{4} \alpha_2 (1 - O(\alpha_2^{1/3})).$$

However, the exact energy $e(\alpha)$ is still not known, and in fact a recent conjecture [CLR17, CDLR19] in the context of a natural approximation, known as **average-field theory** (see [LR15]), suggests that $e(\alpha) \approx (2\sqrt{\pi}/3)2\pi|\alpha|$ for small α , and would thus imply that the

simple linear interpolation $e(\alpha) = 2\pi\alpha_2$ (i.e. $C_1 = C_2 = 2\pi$) between bosons and fermions cannot hold. Furthermore, the picture might change with an additional attraction between the anyons which promotes clustering. Whether the true energy $e(\alpha)$ could be lower for even-numerator rational α than for odd numerators due to the above form of statistical repulsion is an interesting possibility, discussed in more detail in [Lun17].

Exercise 5.11. *Prove the Poincaré inequality (5.28) for functions $u \in H^1([0, \pi])$ subject to the semi-periodic boundary condition (5.27).*

Note that the self-adjoint operator corresponding to the form (5.28) is $D^2 = -\partial_\varphi^2$, with $D = -i\partial_\varphi$ defined as a self-adjoint operator on $L^2([0, \pi])$ with the b.c. (5.27). Then the natural domain of D^2 is the space of functions $u \in H^2([0, \pi])$ satisfying both

$$u(\pi) = e^{i\pi\beta_0}u(0) \quad \text{and} \quad u'(\pi) = e^{i\pi\beta_0}u'(0).$$

6. THE LIEB–THIRRING INEQUALITY

In Section 4 we found that the kinetic energy of an arbitrary L^2 -normalized N -body state $\Psi \in \mathcal{Q}(\hat{T}) = H^1(\mathbb{R}^{dN})$ is bounded from below by (as usual we assume $\hbar^2/(2m) = 1$)

$$T[\Psi] := \left\langle \Psi, \sum_{j=1}^N (-\Delta_j) \Psi \right\rangle \geq G_d N^{-2/d} \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d},$$

which encodes the uncertainty principle by yielding an increase in the kinetic energy for localized densities, but unfortunately becomes overall very weak with $N \rightarrow \infty$. It turns out however that if one restricts to fermionic, i.e. antisymmetric, states $\Psi \in \mathcal{H}_{\text{asym}}$, then this inequality can be improved to

$$T[\Psi] \geq K_d \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d}, \quad (6.1)$$

with a constant $K_d > 0$ that is independent of N . This **fermionic kinetic energy inequality**, which encodes *both* the uncertainty principle *and* the exclusion principle, is also known as a **Lieb–Thirring inequality** and it was introduced by Lieb and Thirring in 1975 [LT75, LT76] in order to give a new and drastically simplified proof of stability of matter, as compared to the original *tour-de-force* proof due to Dyson and Lenard in 1967.

We will apart from proving the celebrated inequality (6.1) for fermions also prove that the assumption on antisymmetry, i.e. the Pauli principle, may be replaced by a strong enough repulsive interaction which then effectively imposes an exclusion principle on the states Ψ as discussed in the previous chapter. In particular, for an inverse-square pair interaction $W(\mathbf{x}) = \beta|\mathbf{x}|^{-2}$, and for any $\Psi \in H^1(\mathbb{R}^{dN})$ (hence also for bosons $\Psi \in \mathcal{H}_{\text{sym}}$ or distinguishable particles), the following Lieb–Thirring-type inequality holds:

$$T[\Psi] + W[\Psi] \geq K_d(\beta) \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d}, \quad (6.2)$$

with a constant $K_d(\beta) > 0$ for any $\beta > 0$. Also other forms of LT inequalities are valid if for instance there is some local statistical repulsion, such as for anyons in two dimensions.

6.1. One-body and Schrödinger formulations. Note that for a fermionic basis state $\Psi = u_1 \wedge u_2 \wedge \dots \wedge u_N$, i.e. a simple Slater determinant, where $\{u_j\}_{j=1}^N \subset \mathfrak{H} = L^2(\mathbb{R}^d)$ denotes an orthonormal set of one-body states, we have that (exercise)

$$T[\Psi] = \sum_{j=1}^N \int_{\mathbb{R}^d} |\nabla u_j|^2, \quad (6.3)$$

and furthermore (exercise)

$$\varrho_\Psi(\mathbf{x}) = \sum_{j=1}^N |u_j(\mathbf{x})|^2. \quad (6.4)$$

The inequality (6.1) on such a state then follows straightforwardly from the following simple generalization of the Gagliardo–Nirenberg–Sobolev inequality of Theorem 4.14. This very simple approach to proving Lieb–Thirring inequalities directly by means of the kinetic energy inequality is quite recent and due to Rumin [Rum10, Rum11] (see also e.g. [Sol11, Fra14, FHJN18] for generalizations).

Theorem 6.1 (Kinetic energy inequality). *Given an L^2 -orthonormal set $\{u_j\}_{j=1}^N \subset H^1(\mathbb{R}^d)$, we have that*

$$\sum_{j=1}^N \int_{\mathbb{R}^d} |\nabla u_j(\mathbf{x})|^2 d\mathbf{x} \geq K_d \int_{\mathbb{R}^d} \left(\sum_{j=1}^N |u_j(\mathbf{x})|^2 \right)^{1+\frac{2}{d}} d\mathbf{x},$$

with a constant satisfying $G'_d \leq K_d \leq \min\{G_d, K_d^{\text{cl}}\}$.

Remark 6.2. See Remark 4.15 concerning the constants $G'_d \leq G_d$. The presently known best bound for the optimal constant K_d is $K_d \geq (1.456)^{-2/d} K_d^{\text{cl}}$ [FHJN18], and it is conjectured that $K_d = G_d < K_d^{\text{cl}}$ for $d \leq 2$ while $K_d = K_d^{\text{cl}} < G_d$ for $d \geq 3$ [LT76]. See also [DLL08, Lap12].

Proof. We follow the proof of Theorem 4.14, with the crucial difference that we use the Bessel inequality in the bound corresponding to (4.23). Namely, we have for the orthonormal system of functions $\{u_j\}_j$ that

$$\sum_{j=1}^N \int_{\mathbb{R}^d} |\nabla u_j(\mathbf{x})|^2 d\mathbf{x} = \sum_{j=1}^N \int_0^\infty \int_{\mathbb{R}^d} |u_j^{E,+}(\mathbf{x})|^2 d\mathbf{x} dE,$$

and by the triangle inequality on \mathbb{C}^N ,

$$\sum_{j=1}^N |u_j^{E,+}(\mathbf{x})|^2 \geq \left[\left(\sum_{j=1}^N |u_j(\mathbf{x})|^2 \right)^{1/2} - \left(\sum_{j=1}^N |u_j^{E,-}(\mathbf{x})|^2 \right)^{1/2} \right]^2_+.$$

The bound on the low-energy part is then done using Fourier transform and Bessel's inequality (2.2) (note that $\{\hat{u}_j\}_j$ are also orthonormal by the unitarity of \mathcal{F}) according to

$$\begin{aligned} \sum_{j=1}^N |u_j^{E,-}(\mathbf{x})|^2 &= \sum_{j=1}^N \left| (2\pi)^{-d/2} \int_{\mathbb{R}^d} \mathbb{1}_{\{|\mathbf{p}|^2 \leq E\}} \hat{u}_j(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{x}} d\mathbf{p} \right|^2 \\ &= (2\pi)^{-d} \sum_{j=1}^N \left| \left\langle \hat{u}_j, \mathbb{1}_{\{|\mathbf{p}| \leq E^{1/2}}\}} e^{i\mathbf{p} \cdot \mathbf{x}} \right\rangle \right|^2 \leq (2\pi)^{-d} |B_{E^{1/2}}(0)|, \end{aligned}$$

after which the remainder of the previous proof goes through with the replacement $\|u\| = 1$, and $K_d \geq G'_d$ of (4.21). Also, since for $N = 1$ the inequality is exactly GNS, we cannot have $K_d > G_d$ for the optimal constants. Furthermore, taking as u_j the eigenfunctions of the Dirichlet Laplacian on a cube, we may as $N \rightarrow \infty$ compare to the Weyl asymptotics (5.3), see e.g. [Krö94], and in fact one may thus prove that also $K_d \leq K_d^{\text{cl}}$. \square

Theorem 6.3 (Many-body kinetic energy inequality). *The inequality*

$$\int_{\mathbb{R}^{dN}} |\nabla \Psi|^2 \geq K_d \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d} \tag{6.5}$$

holds for any $\Psi \in H_{\text{asym}}^1((\mathbb{R}^d)^N)$.

Proof. The proof in the many-body case would again be a straightforward modification of the above one-body case, along the lines of Exercise 4.13, if we only knew that the

corresponding partial traces of Ψ are orthonormal. This is the case for pure product states, i.e. Slater determinants (see Exercise 6.1), but not necessarily so for a general Ψ . What we may do instead is to use a diagonalization trick from the abstract theory of density matrices (which goes slightly outside the course, cf. Remark 3.24, but we nevertheless give here for the interested reader). Alternatively, we will find below that the theorem also follows directly from the above one-body theorem together with the equivalence between the kinetic energy and Schrödinger forms of the inequality; Theorem 6.4 and Corollary 6.6.

Given $\Psi \in \mathcal{H}_{\text{asym}}$ we may form the corresponding one-body density matrix $\gamma_\Psi: \mathfrak{H} \rightarrow \mathfrak{H}$, $\mathfrak{H} = L^2(\mathbb{R}^d)$, defined via the integral kernel

$$\begin{aligned} \gamma_\Psi(\mathbf{x}, \mathbf{y}) := & \sum_{j=1}^N \int_{\mathbb{R}^{d(N-1)}} \Psi(\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{x}, \mathbf{x}_{j+1}, \dots, \mathbf{x}_N) \times \\ & \times \overline{\Psi(\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{y}, \mathbf{x}_{j+1}, \dots, \mathbf{x}_N)} \prod_{k \neq j} d\mathbf{x}_k, \end{aligned}$$

which turns out to be a bounded self-adjoint trace-class operator, with $0 \leq \gamma_\Psi \leq \mathbb{1}$ and $\text{Tr} \gamma_\Psi = N$. It may thus be diagonalized,

$$\gamma_\Psi = \sum_{j=1}^{\infty} \lambda_j u_j \langle u_j, \cdot \rangle$$

with $\lambda_j \in [0, 1]$ and $\{u_j\}_j \subset \mathfrak{H}$ orthonormal. Furthermore,

$$\varrho_\Psi(\mathbf{x}) = \gamma_\Psi(\mathbf{x}, \mathbf{x}) = \sum_{j=1}^{\infty} \lambda_j |u_j(\mathbf{x})|^2.$$

Then

$$T[\Psi] = \sum_{j=1}^{\infty} \langle \Psi, (-\Delta_j) \Psi \rangle = \sum_{j=1}^{\infty} \lambda_j \langle u_j, (-\Delta) u_j \rangle = \sum_{j=1}^{\infty} \lambda_j \int_{\mathbb{R}^d} |\nabla u_j|^2 \geq \sum_{j=1}^M \lambda_j \int_{\mathbb{R}^d} |\nabla u_j|^2,$$

for any $M \in \mathbb{N}$. Now we may modify the proof of Theorem 6.1 slightly by attaching $\sqrt{\lambda_j}$ to each u_j (or taking the triangle inequality on \mathbb{C}^M weighted with λ), with

$$\sum_{j=1}^M \left| \langle \sqrt{\lambda_j} \hat{u}_j, v \rangle \right|^2 = \sum_{j=1}^M \lambda_j |\langle \hat{u}_j, v \rangle|^2 \leq \sum_{j=1}^M |\langle \hat{u}_j, v \rangle|^2 \leq \|v\|^2,$$

again by Bessel's inequality for the orthonormal set $\{\hat{u}_j\}$, and $\lambda_j \leq 1$. Thus,

$$T[\Psi] \geq \sum_{j=1}^M \int_{\mathbb{R}^d} \lambda_j |\nabla u_j(\mathbf{x})|^2 d\mathbf{x} \geq K_d \int_{\mathbb{R}^d} \left(\sum_{j=1}^M \lambda_j |u_j(\mathbf{x})|^2 \right)^{1+\frac{2}{d}} d\mathbf{x},$$

and taking $M \rightarrow \infty$ this proves the theorem. \square

Exercise 6.1. Show (6.3), (6.4) and thus that (6.5) holds for all such basis states Ψ immediately by Theorem 6.1.

6.1.1. *Equivalent Schrödinger operator formulation.* A common and indeed very useful equivalent reformulation of the inequality (6.5) is in the form of an operator inequality involving the negative eigenvalues of the one-body Schrödinger operator on \mathbb{R}^d

$$\hat{h} = -\Delta + V.$$

Both of these formulations are referred to as Lieb–Thirring inequalities. We will be a bit more general here, however, allowing to replace the exclusion principle for fermions with a repulsive pair interaction W or some other statistical repulsion. We denote as usual

$$\begin{aligned} T[\Psi] &= \int_{\mathbb{R}^{dN}} |\nabla \Psi|^2 = \int_{\mathbb{R}^{dN}} \sum_{j=1}^N |\nabla_j \Psi|^2, \\ V[\Psi] &= \int_{\mathbb{R}^{dN}} V |\Psi|^2 = \int_{\mathbb{R}^{dN}} \sum_{j=1}^N V(\mathbf{x}_j) |\Psi(\mathbf{x})|^2 dx, \quad \text{and} \\ W[\Psi] &= \int_{\mathbb{R}^{dN}} W |\Psi|^2 = \int_{\mathbb{R}^{dN}} \sum_{1 \leq j < k \leq N} W(\mathbf{x}_j - \mathbf{x}_k) |\Psi(\mathbf{x})|^2 dx, \end{aligned}$$

so that

$$T[\Psi] + V[\Psi] = \sum_{j=1}^N \int_{\mathbb{R}^{dN}} (|\nabla_j \Psi|^2 + V(\mathbf{x}_j) |\Psi|^2) = \sum_{j=1}^N \langle \Psi, (-\Delta_j + V(\mathbf{x}_j)) \Psi \rangle = \sum_{j=1}^N \langle \Psi, \hat{h}_j \Psi \rangle.$$

Theorem 6.4 (Lieb–Thirring inequalities). *There is an equivalence between **exclusion-kinetic energy inequalities** of the form*

$$T[\Psi] + W[\Psi] \geq K_d(W) \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d}, \quad (6.6)$$

and inequalities for Schrödinger operators of the form

$$T[\Psi] + V[\Psi] + W[\Psi] \geq -L_d(W) \int_{\mathbb{R}^d} |V_-|^{1+d/2}, \quad (6.7)$$

with the relationship between the constants

$$L_d(W) = \frac{2}{d+2} \left(\frac{d}{d+2} \right)^{d/2} K_d(W)^{-d/2}. \quad (6.8)$$

In the above, the interaction W may be replaced by a restriction of the domain of \hat{T} such as to $H_{\text{asym}(q)}^1$, or by a different many-body operator such as \hat{T}_α for anyons.

Remark 6.5. For $N = 1$ (for which $W = 0$ and $\mathcal{H} = \mathcal{H}_{\text{sym}} = \mathcal{H}_{\text{asym}}$) the equivalence is Theorem 4.19 concerning only the uncertainty principle.

Proof. The proof is completely analogous to that of Theorem 4.19, namely, assuming that (6.6) holds, we obtain by Hölder and optimization

$$\begin{aligned} T[\Psi] + W[\Psi] + V[\Psi] &= T[\Psi] + W[\Psi] + \int_{\mathbb{R}^d} |V_+| \varrho_\Psi - \int_{\mathbb{R}^d} |V_-| \varrho_\Psi \\ &\geq K_d \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d} - \left(\int_{\mathbb{R}^d} |V_-|^{1+d/2} \right)^{2/(d+2)} \left(\int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d} \right)^{d/(d+2)} \\ &\geq -L_d \int_{\mathbb{R}^d} |V_-|^{1+d/2}. \end{aligned}$$

On the other hand, if (6.7) holds, then by taking the one-body potential $V(\mathbf{x}) := -c\varrho_\Psi^{2/d}$ we obtain that

$$\begin{aligned} T[\Psi] + W[\Psi] &= T[\Psi] + W[\Psi] + V[\Psi] - V[\Psi] \geq -L_d \int_{\mathbb{R}^d} |V_-|^{1+d/2} - \int_{\mathbb{R}^d} V \varrho_\Psi \\ &= \left(c - c^{1+d/2} L_d \right) \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d}, \end{aligned}$$

which after optimization in $c > 0$ again yields (6.6). \square

Since for fermions $\Psi \in H_{\text{asym}}^1(\mathbb{R}^{dN})$ (with $W = 0$) one has

$$\inf_{\|\Psi\|=1} (T[\Psi] + V[\Psi]) = \sum_{k=0}^{N-1} \lambda_k(\hat{h}),$$

the above equivalence then implies the following inequality for the negative eigenvalues λ_k^- of the one-body Schrödinger operator $\hat{h} = -\Delta + V$ on \mathbb{R}^d :

Corollary 6.6 (Inequality for the sum of Schrödinger eigenvalues). *Let $\{\mu_k\}_{k=0}^\infty$ denote the min-max values of the Schrödinger operator $\hat{h} = -\Delta + V$ on \mathbb{R}^d . Then*

$$\sum_{k=0}^{\infty} |[\mu_k]_-| \leq L_d \int_{\mathbb{R}^d} |V_-(\mathbf{x})|^{1+d/2} d\mathbf{x}. \quad (6.9)$$

Remark 6.7. Note that if the r.h.s. of (6.9) is finite then the bottom of the essential spectrum of \hat{h} must satisfy $\inf \sigma_{\text{ess}}(\hat{h}) \geq 0$, because otherwise all $\mu_k(\hat{h}) \leq \inf \sigma_{\text{ess}}(\hat{h}) < 0$ and thus $\sum_{k=0}^{\infty} |[\mu_k]_-| = \infty$. It follows that the negative min-max values are actually eigenvalues and hence that (6.9) is an inequality for the sum of negative eigenvalues of \hat{h} .

In the spectral theory literature it is usually this inequality that one refers to as the Lieb–Thirring inequality. Also note that it can be generalized to other powers of the eigenvalues as well as to other powers of the Laplacian, including fractional [LS10, Lap12].

Proof. Let $n \leq D := \dim P_{(-\infty, 0)}^{\hat{h}} \mathfrak{H}$ be finite, and denote by $\{u_k\}_{k=0}^{n-1}$ an orthonormal sequence of $C_c^2(\mathbb{R}^d)$ functions corresponding to n lowest negative min-max values $\tilde{\mu}_k := \langle u_k, \hat{h} u_k \rangle$ (approximating μ_k), and $\varrho(\mathbf{x}) := \sum_{k=0}^{n-1} |u_k(\mathbf{x})|^2$. The one-body kinetic energy

inequality of Theorem 6.1 then yields

$$\begin{aligned} -\sum_{k=0}^{n-1} |\tilde{\mu}_k| &= \sum_{k=0}^{n-1} \langle u_k, \hat{h}u_k \rangle = \sum_{k=0}^{n-1} \int_{\mathbb{R}^d} (|\nabla u_k|^2 + V\varrho) \\ &\geq K_d \int_{\mathbb{R}^d} \varrho^{1+2/d} - \int_{\mathbb{R}^d} |V_-|\varrho \geq -L_d \int_{\mathbb{R}^d} |V_-|^{1+d/2}, \end{aligned}$$

where we again estimated by Hölder and optimized as in Theorem 6.4. Taking $n \rightarrow D$ and using that the bound is uniform in the approximation $\tilde{\mu}_k \rightarrow \mu_k$, this proves (6.9). \square

Given the inequality (6.9), one obtains the lower bound

$$\inf_{\substack{\Psi \in \mathcal{H}_{\text{asym}} \\ \|\Psi\|=1}} (T[\Psi] + V[\Psi]) = \sum_{k=0}^{N-1} \lambda_k(\hat{h}) \geq -\sum_{k=0}^{D-1} |\lambda_k^-(\hat{h})| \geq -L_d \int_{\mathbb{R}^d} |V_-|^{1+d/2},$$

which by the equivalence of Theorem 6.4 proves the many-body kinetic energy inequality of Theorem 6.3.

Corollary 6.8 (LT with weaker exclusion). *For any $\Psi \in H_{\text{asym}(q)}^1((\mathbb{R}^d)^N)$, the exclusion-kinetic energy inequality*

$$\int_{\mathbb{R}^{dN}} |\nabla \Psi|^2 \geq q^{-2/d} K_d \int_{\mathbb{R}^d} \varrho_{\Psi}^{1+2/d}$$

holds, and is equivalent to the uniform bound

$$T[\Psi] + V[\Psi] \geq -qL_d \int_{\mathbb{R}^d} |V_-|^{1+d/2}.$$

Proof. One may use the relationship $L_d(\text{asym}(q)) = qL_d(\text{asym}(1)) = qL_d$, following from

$$\inf_{\substack{\Psi \in \mathcal{H}_{\text{asym}(q)} \\ \|\Psi\|=1}} (T[\Psi] + V[\Psi]) = q \sum_{k=0}^{N/q-1} \lambda_k(\hat{h}),$$

and hence $K_d(\text{asym}(q)) = q^{-2/d} K_d(\text{asym}(1)) = q^{-2/d} K_d$ by the correspondence (6.8). \square

6.2. Local approach to Lieb–Thirring inequalities. The above formulations of LT were global in the sense that they always involved the full one-body configuration space \mathbb{R}^d . We shall now consider a local approach to proving LT inequalities, which was first developed in [LS13a] for anyons, and has since been generalized in various directions, including point-interacting fermions [FS12], other types of generalized statistics [LS13b, LS14], inhomogeneously scaling repulsive interactions [LPS15], operators involving fractional powers and critical Hardy terms [LNP16], and most recently gradient corrections to TF [Nam18] as well as vanishing conditions on arbitrary diagonals of the configuration space [LLN19].

6.2.1. Covering lemma. For the local approach it is convenient to use the following lemma which originates in the construction used in [LS13a], and was generalized in [LNP16, Lemmas 9 and 12] and in [Nam18]. The following version includes all those as special cases, though not with the optimal constant.

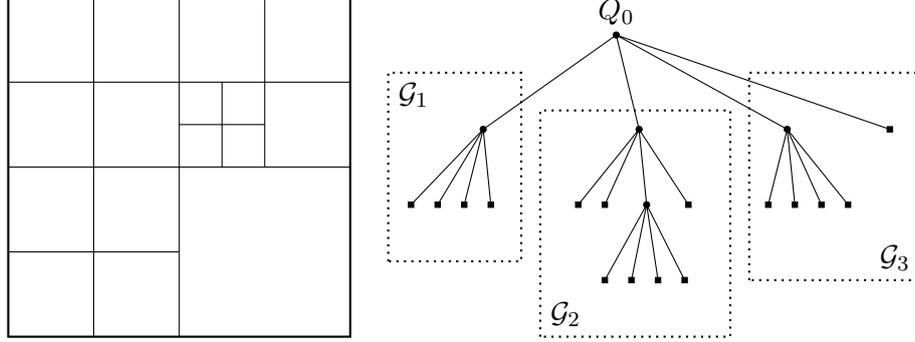


FIGURE 2. Example in $d = 2$ of a division of a square Q_0 and a corresponding tree with three disjoint groups \mathcal{G}_j , together covering all subsquares $Q \in \mathcal{Q}$.

Lemma 6.9 (Covering lemma). *Let Q_0 be a d -cube in \mathbb{R}^d , $d \geq 1$, and let $\Lambda > 0$. Let $0 \leq f \in L^1(Q_0)$ satisfy $\int_{Q_0} f \geq \Lambda > 0$. Then Q_0 can be partitioned into a collection \mathcal{Q} of disjoint sub-cubes $Q \in \mathcal{Q}$, i.e. $Q_0 = \overline{\bigsqcup \mathcal{Q}}$, such that:*

- For all $Q \in \mathcal{Q}$,

$$\int_Q f \leq \Lambda.$$

- For all $\alpha, \beta > 0$ and $\gamma \geq 0$,

$$\sum_{Q \in \mathcal{Q}} \frac{1}{|Q|^\alpha} \left[\left(\int_Q f \right)^\beta - \frac{\Lambda^{\beta-\gamma}}{C_{d,\alpha,\beta}} \left(\int_Q f \right)^\gamma \right] \geq 0, \quad (6.10)$$

where

$$C_{d,\alpha,\beta} := \frac{2^{d(\alpha+\beta+1)}}{2^{d\alpha} - 1}.$$

Proof. Note that if $\int_{Q_0} f = \Lambda$ then there is nothing to prove since $C_{d,\alpha,\beta} > 1$, hence we may assume $\int_{Q_0} f > \Lambda$. We then start by dividing Q_0 into 2^d subcubes Q of equal size, $|Q| = 2^{-d}|Q_0|$, and consider the mass $\int_Q f$ on each such subcube. If $\int_Q f \leq \Lambda$ we do nothing, while if $\int_Q f > \Lambda$ then we may iterate the procedure on Q and divide that cube into 2^d smaller cubes, and so on. This procedure stops after finitely many iterations since f is integrable. We may organize the resulting divisions of cubes into a 2^d -ary tree rooted at Q_0 and with the leaves of the tree representing the resulting disjoint cubes Q that form the sought collection \mathcal{Q} , with $\cup_{Q \in \mathcal{Q}} \bar{Q} = Q_0$ and $\int_Q f \leq \Lambda$. See Figure 2 for an example.

Moreover, we note that the cubes $Q \in \mathcal{Q}$ may be distributed into a finite number of disjoint groups $\mathcal{G} \subseteq \mathcal{Q}$, such that in each group:

- There is a smallest size of cubes in \mathcal{G} , denoted $m := \min_{Q \in \mathcal{G}} |Q|$, and the total mass of such cubes is

$$\sum_{Q \in \mathcal{G}: |Q|=m} \int_Q f \geq \Lambda. \quad (6.11)$$

- There are at most 2^d cubes in \mathcal{G} of every given size.

Such a grouping may be constructed for example by starting with each collection of 2^d leaves which stem from a final split of a cube with $\int_Q f > \Lambda$, and then add leaves to the group by going back in the tree (arbitrarily many times, possibly all the way to the root Q_0) and then one step forward. Note that all leaves will then be covered by at least one such group, and if several, we may choose one arbitrarily.

Now, consider an arbitrary group \mathcal{G} . Because of (6.11), there must be at least one cube $Q \in \mathcal{G}$ with $|Q| = m$ and $\int_Q f \geq \Lambda/2^d$. Hence,

$$\max_{\substack{Q \in \mathcal{G} \\ |Q|=m}} \frac{1}{|Q|^\alpha} \left(\int_Q f \right)^\beta \geq \frac{1}{m^\alpha} \left(\frac{\Lambda}{2^d} \right)^\beta = \frac{\Lambda^\beta}{2^{d\beta} m^\alpha}.$$

Furthermore,

$$\sum_{Q \in \mathcal{G}} \frac{1}{|Q|^\alpha} \left(\int_Q f \right)^\gamma \leq \sum_{k=0}^{\infty} \sum_{\substack{Q \in \mathcal{G} \\ |Q|=m2^{dk}}} \frac{1}{|Q|^\alpha} \Lambda^\gamma \leq \sum_{k=0}^{\infty} \frac{2^d \Lambda^\gamma}{m^\alpha 2^{dk\alpha}} = \frac{2^d \Lambda^\gamma}{m^\alpha} \frac{1}{1 - 2^{-d\alpha}} = \frac{C_{d,\alpha,\beta}}{\Lambda^{\beta-\gamma}} \frac{\Lambda^\beta}{2^{d\beta} m^\alpha},$$

which proves (6.10) on the group \mathcal{G} , and since every cube $Q \in \mathcal{Q}$ belongs to some group, therefore also the lemma. \square

One obtains from this also the following version, which was proven directly and with a slightly different constant in [LNP16, Lemma 12]:

Corollary 6.10 (Weaker exclusion version). *Under the same conditions as in Lemma 6.9, the cube Q_0 may be partitioned into a finite collection \mathcal{Q} of disjoint sub-cubes $Q \in \mathcal{Q}$, such that:*

- For all $Q \in \mathcal{Q}$,

$$\int_Q f \leq \Lambda.$$

- For any $q \geq 0$,

$$\sum_{Q \in \mathcal{Q}} \frac{1}{|Q|^\alpha} \left(\left[\int_Q f - q \right]_+ - b \int_Q f \right) \geq 0, \quad (6.12)$$

where

$$b := 1 - \frac{q}{\Lambda} \frac{2^{d(\alpha+2)}}{2^{d\alpha} - 1}. \quad (6.13)$$

Proof. Note that for any collection \mathcal{Q} of cubes Q

$$\begin{aligned} \sum_{Q \in \mathcal{Q}} \frac{1}{|Q|^\alpha} \left(\left[\int_Q f - q \right]_+ - b \int_Q f \right) &\geq \sum_{Q \in \mathcal{Q}} \frac{1}{|Q|^\alpha} \left((1-b) \int_Q f - q \right) \\ &= (1-b) \sum_{Q \in \mathcal{Q}} \frac{1}{|Q|^\alpha} \left(\int_Q f - \frac{q/\Lambda}{1-b} \Lambda \right). \end{aligned} \quad (6.14)$$

By choosing \mathcal{Q} as in Lemma 6.9, with $\beta = 1$ and $\gamma = 0$, the r.h.s. of (6.14) is non-negative if $b \leq 1$ and if

$$\frac{q/\Lambda}{1-b} = C_{d,\alpha,1}^{-1} = \frac{2^{d\alpha} - 1}{2^{d(\alpha+2)}},$$

that is (6.13). This proves (6.12) (the inequality is trivially true for $b \leq 0$). \square

Exercise 6.2. *Extend the covering lemma to a split into k^d subcubes, with $k \geq 2$. (One practical usefulness of this version for $k = 3$ (or any k odd) is that there is always a cube in \mathcal{Q} whose centerpoint coincides with the centerpoint of Q_0 .)*

6.2.2. *Local proof of LT for fermions.* Let us now use the above covering lemma to prove the fermionic LT inequality of Theorems 6.3 and 6.8 directly by means of the local formulations of the uncertainty and the exclusion principle, although with a weaker constant.

Namely, take $\Psi \in H^1_{\text{asym}(q)}(\mathbb{R}^{dN})$, and recall that for any partition \mathcal{P} of \mathbb{R}^d into cubes Q we have by the local uncertainty principle (4.44) that

$$T[\Psi] = \sum_{Q \in \mathcal{P}} T^Q[\Psi] \geq \sum_{Q \in \mathcal{P}} \left(C_1 \frac{\int_Q \varrho_\Psi^{1+2/d}}{(\int_Q \varrho_\Psi)^{2/d}} - C_2 \frac{\int_Q \varrho_\Psi}{|Q|^{2/d}} \right), \quad (6.15)$$

for some positive constants $C_1, C_2 > 0$, and that the local exclusion principle of Lemma 5.7 yields

$$T^Q[\Psi] \geq \frac{\pi^2}{|Q|^{2/d}} \left[\int_Q \varrho_\Psi - q \right]_+. \quad (6.16)$$

By the GNS inequality on the full space,

$$T[\Psi] \geq G_d N^{-2/d} \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d},$$

we see that $\int_{\mathbb{R}^d \setminus Q_0} \varrho_\Psi^{1+2/d}$ can be made arbitrarily small by taking some large enough cube Q_0 , and thus in a standard approximation argument we may in fact assume $\text{supp } \Psi \subseteq Q_0^N$.

We then take a partition $\mathcal{P} = \mathcal{Q}$ of Q_0 according to Corollary 6.10, and combine the energies (6.15) and (6.16) with $T = \varepsilon T + (1 - \varepsilon)T$ and an arbitrary $\varepsilon \in [0, 1]$, to obtain

$$\begin{aligned} T[\Psi] &\geq \sum_{Q \in \mathcal{Q}} \left(\varepsilon C_1 \frac{\int_Q \varrho_\Psi^{1+2/d}}{(\int_Q \varrho_\Psi)^{2/d}} - \varepsilon C_2 \frac{\int_Q \varrho_\Psi}{|Q|^{2/d}} + (1 - \varepsilon) \frac{\pi^2}{|Q|^{2/d}} \left[\int_Q \varrho_\Psi - q \right]_+ \right) \\ &\geq \sum_{Q \in \mathcal{Q}} \left(\varepsilon C_1 \frac{\int_Q \varrho_\Psi^{1+2/d}}{\Lambda^{2/d}} + ((1 - \varepsilon)\pi^2 b - \varepsilon C_2) \frac{\int_Q \varrho_\Psi}{|Q|^{2/d}} \right), \end{aligned}$$

with $b = 1 - \frac{4}{3}4^d q/\Lambda$ (here $\alpha = 2/d$). Taking $\Lambda = \frac{8}{3}4^d q$ so that $b = 1/2$, and $\varepsilon = \pi^2/(4C_2)$, the last term becomes nonnegative and

$$T[\Psi] \geq Cq^{-2/d} \sum_Q \int_Q \varrho_\Psi^{1+2/d} = Cq^{-2/d} \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d},$$

which proves the theorem. \square

6.2.3. *Local proof of LT for inverse-square repulsion.* Using the above local approach we may also prove the Lieb–Thirring inequality (6.2) for the repulsive pair potential $W_\beta(\mathbf{x}) = \beta|\mathbf{x}|^{-2}$. In this case the natural form domain to be considered is

$$\mathcal{H}_{d,N}^1 := \left\{ \Psi \in H^1(\mathbb{R}^{dN}) : \sum_{1 \leq j < k \leq N} \int_{\mathbb{R}^{dN}} \frac{|\Psi(\mathbf{x})|^2}{|\mathbf{x}_j - \mathbf{x}_k|^2} d\mathbf{x} < \infty \right\}, \quad (6.17)$$

and $0 \leq T[\Psi] + W_\beta[\Psi] < \infty$ for such $\Psi \in \mathcal{H}_{d,N}^1$. The following theorem was proved in [LPS15] (see also [LS14] concerning $d = 1$ and the Calogero–Sutherland model; cf. Section 4.2.3) and generalized to fractional kinetic energy operators in [LNP16]:

Theorem 6.11 (BLT with inverse-square repulsion). *For any $d \geq 1$, $\beta > 0$ there exists a constant $K_d(\beta) > 0$ such that for any $N \geq 1$ and $\Psi \in \mathcal{H}_{d,N}^1$, the exclusion-kinetic energy inequality*

$$T[\Psi] + W_\beta[\Psi] \geq K_d(\beta) \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d} \quad (6.18)$$

holds. Furthermore, for any external one-body potential $V: \mathbb{R}^d \rightarrow \mathbb{R}$,

$$T[\Psi] + V[\Psi] + W_\beta[\Psi] \geq -L_d(\beta) \int_{\mathbb{R}^d} |V_-|^{1+d/2}, \quad (6.19)$$

with the correspondence (6.8) between the constants.

Remark 6.12. The domain $\mathcal{H}_{d,N}^1$ imposes no symmetry on the wave function Ψ , but in fact it may be shown [LS10, Corollary 3.1] that the minimizers of the l.h.s. of (6.18) respectively (6.19) must nevertheless be positive and symmetric, i.e. *bosonic*. We will therefore refer to such an inequality as an (interacting) **bosonic Lieb–Thirring (BLT) inequality**.

Remark 6.13. The behavior of the optimal constant $K_d(\beta)$ in (6.18) as a function of β was discussed in [LNP16, Section 3.5]. One has for all $d \geq 1$ that $K_d(\beta)$ is monotone increasing and concave, and

$$C_d \min\{1, \beta^{2/d}\} \leq K_d(\beta) \leq G_d,$$

for some constant $C_d > 0$, while for

$$\begin{aligned} d = 1: & \quad \lim_{\beta \rightarrow 0} K_1(\beta) = K_1 > 0, \\ d = 2: & \quad \lim_{\beta \rightarrow 0} K_2(\beta) = 0, \\ d \geq 3: & \quad K_d(\beta) \sim \beta^{2/d} \text{ as } \beta \rightarrow 0, \end{aligned}$$

where K_1 is the usual *fermionic* LT constant for $d = 1$. This is because $\mathcal{H}_{1,N}^1 = H_0^1(\mathbb{R}^N \setminus \Delta)$ by the Hardy inequality of Theorem 4.11, and due to our remarks on symmetry as we may multiply the function by a phase (see Section 5.1.2). It is furthermore conjectured that $\lim_{\beta \rightarrow \infty} K_d(\beta) = G_d$ for all $d \geq 1$, and hence that the conjecture on the optimal constant in the fermionic LT (Remark 6.2) for $d = 1$ is equivalent to proving that $K_1(\beta)$ is constant in β . See also [LLN19] for further details concerning $\beta \rightarrow 0$ and recent generalizations.

Proof. We proceed similarly to the previous proof, starting from the same formulation of the local uncertainty principle (6.15). However, (6.16) is now replaced by Lemma 5.10:

$$(T + W_\beta)^Q[\Psi] \geq \frac{1}{2} e_2(Q; W_\beta) \left(\int_Q \varrho_\Psi - 1 \right)_+, \quad (6.20)$$

with $e_2(Q; W_\beta) \geq \beta d^{-1} |Q|^{-2/d}$ by (5.16). Thus, we may just take $q = 1$ and replace π^2 with $\beta/(2d)$ in the previous proof, to obtain

$$T[\Psi] + W_\beta[\Psi] \geq \sum_{Q \in \mathcal{Q}} \left(\varepsilon C_1 \frac{\int_Q \varrho_\Psi^{1+2/d}}{\Lambda^{2/d}} + \left((1 - \varepsilon) \frac{\beta b}{2d} - \varepsilon C_2 \right) \frac{\int_Q \varrho_\Psi}{|Q|^{2/d}} \right) \geq \varepsilon C \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d},$$

with Λ fixed and $\varepsilon \sim \beta$ as $\beta \rightarrow 0$.

In order to get an improved dependence for small β , one may instead use the convexity in n of the bound $e_n(|Q|; W_\beta) \geq \frac{\beta n(n-1)_+}{2d|Q|^{2/d}}$ to replace (6.20) by the improved local exclusion principle

$$(T + W_\beta)^Q[\Psi] \geq \frac{\beta}{2d|Q|^{2/d}} \left(\left(\int_Q \varrho_\Psi \right)^2 - \int_Q \varrho_\Psi \right)_+.$$

Then, by Lemma 6.9 with $\alpha = 2/d$, $\beta = 2$ (different β), and $\gamma = 1$,

$$\begin{aligned} T[\Psi] + W_\beta[\Psi] &\geq \sum_{Q \in \mathcal{Q}} \left(\varepsilon C_1 \frac{\int_Q \varrho_\Psi^{1+2/d}}{\Lambda^{2/d}} + \left((1-\varepsilon) \frac{\beta}{2d} \frac{\Lambda}{C_{d,2/d,2}} - (1-\varepsilon) \frac{\beta}{2d} - \varepsilon C_2 \right) \frac{\int_Q \varrho_\Psi}{|Q|^{2/d}} \right) \\ &\geq \varepsilon C_1 \Lambda^{-2/d} \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d}, \end{aligned}$$

with suitable fixed $\varepsilon > 0$ and $\Lambda \sim \beta^{-1}$ as $\beta \rightarrow 0$. \square

6.2.4. Local proof of LT for anyons. We may furthermore extend the Lieb–Thirring inequality straightforwardly to anyons in two dimensions using their local exclusion principle given in Lemma 5.16 [LS18]. Recall the periodization of the statistics parameter $\alpha_2 = \min_{q \in \mathbb{Z}} |\alpha - 2q| \in [0, 1]$.

Theorem 6.14 (LT for anyons). *There exists a constant $K_2 > 0$ such that for any $\alpha \in \mathbb{R}$, any $N \geq 1$ and $\Psi \in \mathcal{Q}(\hat{T}_\alpha)$, the exclusion-kinetic energy inequality*

$$T_\alpha[\Psi] \geq K_2 \alpha_2 \int_{\mathbb{R}^2} \varrho_\Psi^2$$

holds. Furthermore, for any external one-body potential $V: \mathbb{R}^2 \rightarrow \mathbb{R}$,

$$T_\alpha[\Psi] + V[\Psi] \geq -L_2 \alpha_2^{-1} \int_{\mathbb{R}^d} |V_-|^2,$$

with the correspondence (6.8) between the constants K_2 and L_2 .

Proof. For local uncertainty we use the diamagnetic inequality of Lemma 5.15,

$$T_\alpha[\Psi] \geq T_{\alpha=0}[|\Psi|] = \sum_{Q \in \mathcal{P}} T_{\alpha=0}^Q[|\Psi|] \geq \sum_{Q \in \mathcal{P}} \left(C_1 \frac{\int_Q \varrho_\Psi^2}{\int_Q \varrho_\Psi} - C_2 \frac{\int_Q \varrho_\Psi}{|Q|} \right).$$

The proof then goes through exactly as in Section 6.2.2, replacing π^2 in (6.16) with $c(\alpha) \geq \alpha_2/12$ from Lemma 5.16. \square

6.2.5. Local LT with semiclassical constant. Recently, Nam has considered improvements w.r.t. the constant in the local approach, getting arbitrarily close to the semiclassical one, to the cost of a gradient error term [Nam18]. Namely, using the Weyl asymptotics on cubes one may first prove the following:

Lemma 6.15 (Local density approximation). *Given any $\Psi \in H_{\text{asym}}^1((\mathbb{R}^d)^N)$ and d -cube Q_0 such that $\int_{Q_0} \varrho_\Psi \geq \Lambda > 0$, there exists a partition \mathcal{Q} of Q_0 into sub-cubes Q such that*

$\int_Q \varrho_\Psi \leq \Lambda$ and

$$\int_{\mathbb{R}^{dN}} |\nabla \Psi|^2 \geq K_d^{\text{cl}} (1 - C_d \Lambda^{-1/d}) \sum_{Q \in \mathcal{Q}} |Q| \left(\frac{\int_Q \varrho_\Psi}{|Q|} \right)^{1+2/d}, \quad (6.21)$$

where C_d is a constant depending only on d .

Proof. The Weyl asymptotics (5.3) for the sum of Laplacian eigenvalues on a cube Q can be rigorously justified with a uniform lower bound (see e.g. [Krö94])

$$e_N(|Q|; \text{asym}) = \sum_{k=0}^{N-1} \lambda_k(-\Delta_Q^N) \geq \frac{K_d^{\text{cl}}}{|Q|^{2/d}} \left(N^{1+2/d} - CN^{1+1/d} \right)_+$$

for some constant $C > 0$ and all $N \in \mathbb{N}$. Using that the r.h.s. is convex in $N > 0$, one may then also prove the following improvement of the local exclusion principle of Lemma 5.7:

$$T^Q[\Psi] \geq \frac{K_d^{\text{cl}}}{|Q|^{2/d}} \left(\left(\int_Q \varrho_\Psi \right)^{1+2/d} - C \left(\int_Q \varrho_\Psi \right)^{1+1/d} \right)_+.$$

Now, applying Lemma 6.9 in the second term with $\alpha = 2/d$, $\beta = 1 + 2/d$ and $\gamma = 1 + 1/d$, one obtains

$$T[\Psi] \geq \sum_{Q \in \mathcal{Q}} T^Q[\Psi] \geq \sum_{Q \in \mathcal{Q}} \frac{K_d^{\text{cl}}}{|Q|^{2/d}} \left(\left(\int_Q \varrho_\Psi \right)^{1+2/d} - C \frac{C_{d,\alpha,\beta}}{\Lambda^{1/d}} \left(\int_Q \varrho_\Psi \right)^{1+2/d} \right),$$

for the corresponding partition \mathcal{Q} of Q_0 , which proves (6.21). \square

Lemma 6.15 is a local density approximation for the Thomas-Fermi energy. In fact, Nam proved the following consequence, which shows that if the density is sufficiently constant then one indeed obtains the Thomas-Fermi energy as a lower bound, with the semiclassical constant:

Theorem 6.16 (LT with gradient correction). *There exists a constant $C_d > 0$ s.t. the inequality*

$$\int_{\mathbb{R}^{dN}} |\nabla \Psi|^2 \geq (1 - \varepsilon) K_d^{\text{cl}} \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d} - \frac{C_d}{\varepsilon^{3+4/d}} \int_{\mathbb{R}^d} |\nabla \sqrt{\varrho_\Psi}|^2$$

holds for any $\varepsilon > 0$ and $\Psi \in H_{\text{asym}}^1((\mathbb{R}^d)^N)$.

See also [LLS19] for recent related results concerning the electron gas.

6.3. Some direct applications of LT. As a direct application of the above kinetic energy inequalities one may consider the ground-state energy of a system of N particles with a given external potential V . Namely, given a bound of the form (6.6), one may estimate the N -body energy in terms of the density,

$$T[\Psi] + V[\Psi] + W[\Psi] \geq \int_{\mathbb{R}^d} \left(K_d(W) \varrho_\Psi^{1+2/d}(\mathbf{x}) + V \varrho_\Psi(\mathbf{x}) \right) d\mathbf{x} =: \tilde{\mathcal{E}}[\varrho_\Psi], \quad (6.22)$$

with $\varrho_\Psi \in L^{1+2/d}(\mathbb{R}^d; \mathbb{R}_+)$, $\int_{\mathbb{R}^d} \varrho_\Psi = N$, and therefore the simple minimization problem

$$E_0(N) \geq \inf \left\{ \tilde{\mathcal{E}}[\varrho] : \varrho \in L^{1+2/d}(\mathbb{R}^d; \mathbb{R}_+), \int_{\mathbb{R}^d} \varrho = N \right\}.$$

Another bound for E_0 is given directly in terms of an integral of V_- by (6.7), but note that the above bound is also valid for arbitrary, even non-negative, one-body potentials V .

Example 6.17 (The homogeneous gas). We model the case of a homogeneous gas on a finite domain $\Omega \subseteq \mathbb{R}^d$ by formally taking for the one-body potential a flat external trap with infinite walls,

$$V(\mathbf{x}) = \begin{cases} 0, & \text{on } \Omega, \\ +\infty, & \text{on } \Omega^c. \end{cases}$$

More precisely, we take Dirichlet boundary conditions, $\Psi \in H_0^1(\Omega^N)$. Then also $\text{supp } \varrho_\Psi \subseteq \Omega$, $\int_\Omega \varrho_\Psi = N$, and since we have by Hölder that

$$\tilde{\mathcal{E}}[\varrho] = K_d(W) \int_\Omega \varrho^{1+2/d} \geq K_d(W) |\Omega|^{-2/d} \left(\int_\Omega \varrho \right)^{1+2/d}$$

for any $\varrho \in L^1(\Omega; \mathbb{R}_+)$, we then obtain by (6.22), for the ground state energy per particle of the homogeneous gas with density $\rho = N/|\Omega|$,

$$\frac{E_0(N)}{N} = \inf_{\substack{\Psi \in H_0^1(\Omega^N) \\ \|\Psi\|=1}} \frac{1}{N} (T[\Psi] + V[\Psi] + W[\Psi]) \geq K_d(W) \rho^{2/d}.$$

In the case of fermions (compare Example 5.8) this lower bound will exactly match the correct energy given by the Weyl asymptotics (5.3), even including the conjectured optimal constant $K_d(\text{asym}) \stackrel{\text{conj.}}{=} K_d^{\text{cl}}$ in higher dimensions $d \geq 3$ (see Remark 6.2).

Exercise 6.3 (Harmonic traps). Apply the bound (6.22) to a harmonic oscillator potential $V_{\text{osc}}(\mathbf{x}) = \frac{1}{4}\omega^2|\mathbf{x}|^2$. Show that $\varrho_{\min}(\mathbf{x}) = K_d(W)^{-d/2} \left(\frac{d}{d+2} \right)^{d/2} \left(\lambda - \frac{\omega^2}{4}|\mathbf{x}|^2 \right)_+^{d/2}$ for some constant $\lambda = \lambda(d, N) \sim N^{1/d}$. Compute a lower bound $\tilde{\mathcal{E}}[\varrho_{\min}] \sim N^{1+1/d}$ to the energy, and compare to Exercise 5.1 when W is replaced by antisymmetry.

7. THE STABILITY OF MATTER

Recall from Section 3.6.1 that we consider the following many-body Hamiltonian for matter consisting of N particles of one type ('electrons') and M particles of another type ('nuclei') moving in \mathbb{R}^3 :

$$\hat{H}^{N,M} := \sum_{j=1}^N \frac{\hbar^2}{2m_e} (-\Delta_{\mathbf{x}_j}) + \sum_{k=1}^M \frac{\hbar^2}{2m_n} (-\Delta_{\mathbf{R}_k}) + W_C(\mathbf{x}, \mathbf{R}), \quad (7.1)$$

with the full Coulomb interaction

$$W_C(\mathbf{x}, \mathbf{R}) := \sum_{1 \leq i < j \leq N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} - \sum_{j=1}^N \sum_{k=1}^M \frac{Z}{|\mathbf{x}_j - \mathbf{R}_k|} + \sum_{1 \leq k < l \leq M} \frac{Z^2}{|\mathbf{R}_k - \mathbf{R}_l|}. \quad (7.2)$$

As usual we assume that the electrons have charge -1 and the nuclei charge $Z > 0$, and put $\hbar = 1$ by a change of mass scale. One may also have different masses and charges for the nuclei but we will stick to this technically simplifying assumption here. Furthermore, we could also consider the nuclei to be fixed at the positions $\mathbf{R} = (\mathbf{R}_k)_{k=1}^M$ by formally taking $m_n = +\infty$, or equivalently, just remove their kinetic energy terms in (7.1):

$$\hat{H}^N(\mathbf{R}) := \sum_{j=1}^N \frac{1}{2m_e} (-\Delta_{\mathbf{x}_j}) + W_C(\mathbf{x}, \mathbf{R}). \quad (7.3)$$

Since $\hat{H}^{N,M} \geq \hat{H}^N(\mathbf{R})$ as quadratic forms on $H^1(\mathbb{R}^{3(N+M)})$, obtaining a lower bound for (7.3) which is uniform in \mathbf{R} will then also be valid as a lower bound for $\hat{H}^{N,M}$.

7.1. Stability of the first kind. That the Hamiltonian operators (7.1) and (7.3) are bounded from below, i.e. stability of the *first* kind in the terminology of Definition 3.21, is a simple consequence of the uncertainty principle. Namely, recall the stability of the single hydrogenic atom,

$$-\frac{1}{2m} \Delta_{\mathbb{R}^3} - \frac{Z}{|\mathbf{x}|} \geq -\frac{1}{2} m Z^2, \quad (7.4)$$

which is the sharp lower bound from the ground-state solution (4.35) or, with just a slightly worse constant, from Hardy (4.31) or Sobolev (4.33).

Theorem 7.1 (Stability of the first kind). *For any number of particles $N, M \geq 1$, for any positions of the nuclei $\mathbf{R} \in \mathbb{R}^{3M}$, and for any mass $m_e > 0$ and charge $Z > 0$, we have*

$$\hat{H}^N(\mathbf{R}) \geq -\frac{1}{2} m_e Z^2 N M^2, \quad (7.5)$$

with respect to the form domain $H^1(\mathbb{R}^{3N})$ (with unrestricted symmetry), from which $\hat{H}^N(\mathbf{R})$ extends to a bounded-from-below (uniformly in \mathbf{R}) self-adjoint operator on $\mathcal{H}^N = L^2(\mathbb{R}^{3N})$. Hence,

$$\hat{H}^{N,M} \geq \inf_{\mathbf{R} \in \mathbb{R}^{3M}} \hat{H}^N(\mathbf{R}) \geq -\frac{1}{2} m_e Z^2 N M^2, \quad (7.6)$$

in the sense of forms on $H^1(\mathbb{R}^{3(N+M)})$, from which $\hat{H}^{N,M}$ extends to a bounded-from-below self-adjoint operator on $\mathcal{H}^{N,M} = L^2(\mathbb{R}^{3(N+M)})$.

Proof. Let us simply throw away the positive terms in W_C and write in terms of forms

$$\hat{H}^N(\mathbf{R}) \geq \sum_{j=1}^N \sum_{k=1}^M \left[\frac{1}{2m_e M} (-\Delta_{\mathbf{x}_j}) - \frac{Z}{|\mathbf{x}_j - \mathbf{R}_k|} \right] \geq - \sum_{j=1}^N \sum_{k=1}^M \frac{1}{2} m_e M Z^2 = -\frac{1}{2} m_e Z^2 N M^2,$$

by (7.4). This proves (7.5), and by the inequality

$$\left\langle \Psi, \hat{H}^{N,M} \Psi \right\rangle_{L^2(\mathbb{R}^{3(N+M)})} \geq \int_{\mathbb{R}^{3M}} \left\langle \Psi(\cdot, \mathbf{R}), \hat{H}^N(\mathbf{R}) \Psi(\cdot, \mathbf{R}) \right\rangle_{L^2(\mathbb{R}^{3N})} d\mathbf{R}$$

applied on arbitrary $\Psi \in H^1(\mathbb{R}^{3(N+M)})$, also (7.6). \square

7.2. Some electrostatics. In order to improve the above bound to a linear one in $N + M$, i.e. prove stability of the second kind, we also need some important results on electrostatics.

7.2.1. Baxter's inequality. The main result that we need for the proof of stability is the following inequality due to Baxter [Bax80], which replaces all the $N^2 + NM + M^2$ terms of the full Coulomb interaction (7.2) by only $N + M$ nearest-neighbor terms [LS10, Theorem 5.4]:

Theorem 7.2 (Baxter's inequality). *For any $\mathbf{x} \in \mathbb{R}^{3N}$, $\mathbf{R} \in \mathbb{R}^{3M}$, and $Z \geq 0$ we have*

$$W_C(\mathbf{x}, \mathbf{R}) \geq -(2Z + 1) \sum_{j=1}^N \frac{1}{\text{dist}(\mathbf{x}_j, \mathbf{R})} + \frac{Z^2}{4} \sum_{k=1}^M \frac{1}{\text{dist}(\mathbf{R}_k, \mathbf{R}_{\setminus k})}, \quad (7.7)$$

where $\text{dist}(\mathbf{x}, \mathbf{R}) = \min_{k \in \{1, \dots, M\}} |\mathbf{x} - \mathbf{R}_k|$ and $\text{dist}(\mathbf{R}, \mathbf{R}_{\setminus k}) = \min_{l \in \{1, \dots, k-1, k+2, \dots, M\}} |\mathbf{R} - \mathbf{R}_l|$.

To reach this bound, which is an example of **electrostatic screening**, we first introduce a few basic electrostatic notions. We closely follow [Sei10] and [LS10] in this section.

7.2.2. Coulomb technology and Newton's theorem. Let us consider a general **charge distribution**, that is a signed Borel measure $\mu = \mu_+ - \mu_-$ on \mathbb{R}^3 ($\mu_{\pm} \geq 0$), and its corresponding **Coulomb potential function**

$$\Phi_{\mu}(\mathbf{x}) = \int_{\mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{y}|} d\mu(\mathbf{y}), \quad \mathbf{x} \in \mathbb{R}^3.$$

We also define its **Coulomb self-energy**⁽²⁰⁾

$$D(\mu, \mu) := \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{y}|} d\mu(\mathbf{x}) d\mu(\mathbf{y}) = \frac{1}{2} \int_{\mathbb{R}^3} \Phi_{\mu}(\mathbf{x}) d\mu(\mathbf{x}).$$

Note that for the point charge $\mu = \delta_{\mathbf{x}_0}$ we have $D(\mu, \mu) = \Phi_{\mu}(\mathbf{x}_0) = +\infty$ and indeed we could allow infinite values for charge distributions of definite sign. However, to make these expressions well defined also in the case of indefinite sign we consider the class of measures

$$\mathcal{C} = \left\{ \mu = \mu_+ - \mu_- : \int_{\mathbb{R}^3} \frac{d\mu_{\pm}(\mathbf{x})}{1 + |\mathbf{x}|} < \infty \text{ and } D(\mu_{\pm}, \mu_{\pm}) < \infty \right\}.$$

For two such charge distributions $\mu, \nu \in \mathcal{C}$, their **Coulomb interaction energy** is

$$D(\mu, \nu) := \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{y}|} d\mu(\mathbf{x}) d\nu(\mathbf{y}).$$

⁽²⁰⁾The conventional factor 1/2 matches the conventional symmetrized pair-interaction energy.

Lemma 7.3. *The Coulomb self-energy is positive semidefinite, i.e. $0 \leq D(\mu, \mu) < \infty$ for any $\mu \in \mathcal{C}$, and furthermore the interaction energy is bounded in terms of the self-energy,*

$$D(\mu, \nu)^2 \leq D(\mu, \mu)D(\nu, \nu), \quad \mu, \nu \in \mathcal{C}.$$

Proof. We use that (exercise)

$$\frac{1}{|\mathbf{x} - \mathbf{y}|} = C \int_{\mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{z}|^2} \frac{1}{|\mathbf{y} - \mathbf{z}|^2} d\mathbf{z} \quad (7.8)$$

for some constant $C > 0$ (in fact one may compute $C = \pi^{-3}$). This follows simply by the observation that both sides are functions of $\mathbf{x} - \mathbf{y}$ and scale homogeneously to degree -1 .

Thus, by Fubini,

$$D(\mu, \mu) = \frac{C}{2} \int_{\mathbb{R}^3} \left(\int_{\mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{z}|^2} d\mu(\mathbf{x}) \right)^2 d\mathbf{z} \geq 0,$$

and similarly, by Cauchy-Schwarz,

$$D(\mu, \nu) = \frac{C}{2} \int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{z}|^2} d\mu(\mathbf{x}) \int_{\mathbb{R}^3} \frac{1}{|\mathbf{y} - \mathbf{z}|^2} d\nu(\mathbf{y}) \right] d\mathbf{z} \leq D(\mu, \mu)^{1/2} D(\nu, \nu)^{1/2}.$$

We also have the triangle inequality

$$(D(\mu_+, \mu_+)^{1/2} - D(\mu_-, \mu_-)^{1/2})^2 \leq D(\mu_+ - \mu_-, \mu_+ - \mu_-) \leq (D(\mu_+, \mu_+)^{1/2} + D(\mu_-, \mu_-)^{1/2})^2,$$

and in particular finiteness of $D(\mu, \mu)$ for $\mu \in \mathcal{C}$. \square

Theorem 7.4 (Newton's Theorem). *Let $\mu \in \mathcal{C}$ be rotationally symmetric with respect to the origin (i.e. $\mu(R\Omega) = \mu(\Omega)$ for any rotation $R \in \text{SO}(\mathbb{R}^3)$) and measurable set $\Omega \subseteq \mathbb{R}^3$). Then*

$$\Phi_\mu(\mathbf{x}) = \frac{1}{|\mathbf{x}|} \int_{|\mathbf{y}| \leq |\mathbf{x}|} d\mu(\mathbf{y}) + \int_{|\mathbf{y}| > |\mathbf{x}|} \frac{1}{|\mathbf{y}|} d\mu(\mathbf{y}), \quad \mathbf{x} \in \mathbb{R}^3.$$

Proof. The rotational symmetry of μ carries over to Φ_μ , with

$$\Phi_\mu(\mathbf{x}) = \frac{1}{4\pi} \int_{\mathbb{S}^2} \Phi_\mu(|\mathbf{x}|\boldsymbol{\omega}) d\boldsymbol{\omega} = \int_{\mathbb{R}^3} \frac{1}{4\pi} \int_{\mathbb{S}^2} \frac{1}{||\mathbf{x}|\boldsymbol{\omega} - \mathbf{y}|} d\boldsymbol{\omega} d\mu(\mathbf{y}).$$

We use Fubini and calculate

$$\begin{aligned} \frac{1}{4\pi} \int_{\mathbb{S}^2} \frac{1}{||\mathbf{x}|\boldsymbol{\omega} - \mathbf{y}|} d\boldsymbol{\omega} &= \frac{1}{2} \int_{-1}^1 \frac{1}{\sqrt{|\mathbf{x}|^2 + |\mathbf{y}|^2 - 2|\mathbf{x}||\mathbf{y}|t}} dt \\ &= \frac{1}{2|\mathbf{x}||\mathbf{y}|} \left(\sqrt{|\mathbf{x}|^2 + |\mathbf{y}|^2 + 2|\mathbf{x}||\mathbf{y}|} - \sqrt{|\mathbf{x}|^2 + |\mathbf{y}|^2 - 2|\mathbf{x}||\mathbf{y}|} \right) \\ &= \frac{1}{2|\mathbf{x}||\mathbf{y}|} (|\mathbf{x}| + |\mathbf{y}| - ||\mathbf{x}| - |\mathbf{y}||) = \min \left\{ \frac{1}{|\mathbf{x}|}, \frac{1}{|\mathbf{y}|} \right\}, \end{aligned}$$

which proves the theorem. \square

7.2.3. Basic Electrostatic Inequality. Given distinct points $\mathbf{R}_1, \dots, \mathbf{R}_M \in \mathbb{R}^3$, define their corresponding **Voronoi cells** $\Gamma_1, \dots, \Gamma_M$ as the sets

$$\Gamma_k := \{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x} - \mathbf{R}_k| < |\mathbf{x} - \mathbf{R}_l| \text{ for all } l \neq k\}.$$

Note that $\{\Gamma_k\}$ partitions \mathbb{R}^3 into M disjoint pieces (up to a null set $\cup_k \partial\Gamma_k$), and that each such cell Γ_k is convex, being the intersection of $M - 1$ half-spaces in \mathbb{R}^3 .

Let

$$\Phi(\mathbf{x}) = \sum_{k=1}^M \frac{Z}{|\mathbf{x} - \mathbf{R}_k|} - \frac{Z}{\text{dist}(\mathbf{x}, \mathbf{R})},$$

that is the potential from all the nuclei except the nearest one, that is on each Voronoi cell Γ_k it is the Coulomb potential seen from all nuclei outside Γ_k .

Theorem 7.5 (Basic Electrostatic Inequality). *If $\mu \in \mathcal{C}$ is a charge distribution then*

$$D(\mu, \mu) - \int_{\mathbb{R}^3} \Phi(\mathbf{x}) d\mu(\mathbf{x}) + \sum_{k < l} \frac{Z^2}{|\mathbf{R}_k - \mathbf{R}_l|} \geq \frac{1}{4} \sum_{k=1}^M \frac{Z^2}{\text{dist}(\mathbf{R}_k, \mathbf{R}_{\setminus k})}.$$

Proof. We claim that the second term may be written $-2D(\mu, \nu)$ for some $\nu \in \mathcal{C}$, so that the l.h.s. equals

$$D(\mu - \nu, \mu - \nu) - D(\nu, \nu) + \sum_{k < l} \frac{Z^2}{|\mathbf{R}_k - \mathbf{R}_l|} \geq -D(\nu, \nu) + \sum_{k < l} \frac{Z^2}{|\mathbf{R}_k - \mathbf{R}_l|}. \quad (7.9)$$

To prove the claim and find such ν , note that if $\int_{\mathbb{R}^3} \Phi(\mathbf{x}) d\mu(\mathbf{x}) = 2D(\mu, \nu) = \int_{\mathbb{R}^3} \Phi_\nu(\mathbf{x}) d\mu(\mathbf{x})$ for all $\mu \in \mathcal{C}$ i.e. if $\Phi = \Phi_\nu$ for some $\nu \in \mathcal{C}$, then equivalently $-\Delta\Phi = 4\pi\nu$. Note first that Φ is continuous on \mathbb{R}^3 and moreover since the singularity has been cancelled inside each Γ_k it is smooth and harmonic on $\mathbb{R}^3 \setminus (\cup_k \partial\Gamma_k)$. Hence the measure ν must be supported on the boundaries of the Voronoi cells. We compute for any test function $f \in C_c^\infty(\mathbb{R}^3; \mathbb{R})$

$$\begin{aligned} \int_{\mathbb{R}^3} \Phi(\mathbf{x}) \Delta f(\mathbf{x}) d\mathbf{x} &= \sum_k \int_{\Gamma_k} \Phi \Delta f = \sum_k \int_{\Gamma_k} \nabla \cdot (\Phi \nabla f) - \sum_k \int_{\Gamma_k} \nabla \Phi \cdot \nabla f \\ &= \sum_k \int_{\partial\Gamma_k} \Phi(\mathbf{x}) \nabla f(\mathbf{x}) \cdot \mathbf{n}_k dS - \sum_k \int_{\Gamma_k} \nabla f \cdot \nabla \Phi, \end{aligned}$$

by the divergence theorem, where \mathbf{n}_k denotes the outward unit normal to $\partial\Gamma_k$. The first set of boundary terms vanish by the continuity of Φ and ∇f and the fact that each boundary segment is visited twice with opposite directions of the normal. For the second set of terms we obtain

$$- \int_{\Gamma_k} \nabla f \cdot \nabla \Phi = - \int_{\Gamma_k} \nabla \cdot (f \nabla \Phi) + \int_{\Gamma_k} f \Delta \Phi = - \int_{\partial\Gamma_k} f(\mathbf{x}) \nabla \Phi(\mathbf{x}) \cdot \mathbf{n}_k dS,$$

by the harmonicity of Φ on Γ_k . We have thus on each $\partial\Gamma_k = \partial\Gamma_l$, where l is numbers a neighboring Voronoi cell, actually two terms (and on even smaller measure possibly more terms)

$$\mathbf{n}_k \cdot \nabla \Phi|_{\partial\Gamma_k} + \mathbf{n}_l \cdot \nabla \Phi|_{\partial\Gamma_l} = \mathbf{n}_k \cdot \nabla \frac{-Z}{|\mathbf{x} - \mathbf{R}_k|} + \mathbf{n}_l \cdot \nabla \frac{-Z}{|\mathbf{x} - \mathbf{R}_l|} = -2Z \mathbf{n}_k \cdot \nabla \frac{1}{|\mathbf{x} - \mathbf{R}_k|},$$

that is $\nu = -\frac{1}{4\pi}\Delta\Phi$ is the measure supported on $\cup_k\partial\Gamma_k$ with density

$$-\frac{Z}{2\pi}\mathbf{n}_k \cdot \nabla \frac{1}{|\mathbf{x} - \mathbf{R}_k|} \quad \text{on } \partial\Gamma_k.$$

Moreover, $\nu \geq 0$, because the Voronoi cells Γ_k are convex and thus $\mathbf{n}_k \cdot (\mathbf{x} - \mathbf{R}_k) \geq 0$ for all $\mathbf{x} \in \partial\Gamma_k$.

It remains to compute $D(\nu, \nu)$:

$$D(\nu, \nu) = \frac{1}{2} \int_{\mathbb{R}^3} \Phi(\mathbf{x}) d\nu(\mathbf{x}) = \frac{1}{2} \sum_k \int_{\mathbb{R}^3} \frac{Z}{|\mathbf{x} - \mathbf{R}_k|} d\nu(\mathbf{x}) - \frac{1}{2} \int_{\mathbb{R}^3} \frac{Z}{\text{dist}(\mathbf{x}, \mathbf{R})} d\nu(\mathbf{x}),$$

where

$$\int_{\mathbb{R}^3} \frac{Z}{|\mathbf{x} - \mathbf{R}_k|} d\nu(\mathbf{x}) = Z\Phi_\nu(\mathbf{R}_k) = Z\Phi(\mathbf{R}_k) = \sum_{l \neq k} \frac{Z^2}{|\mathbf{R}_k - \mathbf{R}_l|}$$

exactly matches the last term of (7.9), and

$$\frac{1}{2} \int_{\mathbb{R}^3} \frac{Z}{\text{dist}(\mathbf{x}, \mathbf{R})} d\nu(\mathbf{x}) = - \sum_k \frac{Z^2}{8\pi} \int_{\partial\Gamma_k} \frac{1}{|\mathbf{x} - \mathbf{R}_k|} \mathbf{n}_k \cdot \nabla \frac{1}{|\mathbf{x} - \mathbf{R}_k|} dS,$$

by the definition of the measure ν . Using that $2|\mathbf{x}|^{-1}\nabla|\mathbf{x}|^{-1} = \nabla|\mathbf{x}|^{-2}$ the r.h.s. is

$$- \sum_k \frac{Z^2}{16\pi} \int_{\partial\Gamma_k} \mathbf{n}_k \cdot \nabla \frac{1}{|\mathbf{x} - \mathbf{R}_k|^2} dS = \sum_k \frac{Z^2}{16\pi} \int_{\Gamma_k^c} \Delta \frac{1}{|\mathbf{x} - \mathbf{R}_k|^2} d\mathbf{x}$$

(note that we are now considering the exterior domain). We also compute

$$\Delta \frac{1}{|\mathbf{x} - \mathbf{R}_k|^2} = \frac{2}{|\mathbf{x} - \mathbf{R}_k|^4}$$

and finally estimate the integral

$$\frac{Z^2}{8\pi} \int_{\Gamma_k^c} \frac{d\mathbf{x}}{|\mathbf{x} - \mathbf{R}_k|^4} \geq \frac{Z^2}{8\pi} \int_{z=-\infty}^{\infty} \int_{y=-\infty}^{\infty} \int_{x=D_k}^{\infty} \frac{dx dy dz}{(x^2 + y^2 + z^2)^2} = \frac{Z^2}{8D_k},$$

where $D_k := \text{dist}(\mathbf{R}_k, \partial\Gamma_k) = \frac{1}{2} \min_{l \neq k} |\mathbf{R}_k - \mathbf{R}_l| = \frac{1}{2} \text{dist}(\mathbf{R}_k, \mathbf{R}_{\setminus k})$, and we w.l.o.g. translated to $\mathbf{R}_k = \mathbf{0}$ and rotated part of $\partial\Gamma_k$ to the half-plane parallel to the yz -plane. The remaining three integrals may then be evaluated in cylinder coordinates. \square

7.2.4. Proof of Baxter's inequality. We reduce the original interaction potential W_C to the form of the Basic Electrostatic Inequality by first regularizing the charge distribution of the electrons from points to spherical shells of about the size of the Voronoi cells.

For given $\mathbf{R} = (\mathbf{R}_1, \dots, \mathbf{R}_M) \in \mathbb{R}^{3M}$ and $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^{3N}$ we denote $d_j := \text{dist}(\mathbf{x}_j, \mathbf{R})$ and let

$$\mu_j(d\mathbf{x}) := (\pi d_j^2)^{-1} \delta(|\mathbf{x} - \mathbf{x}_j| - d_j/2) d\mathbf{x},$$

and $\mu := \sum_{j=1}^N \mu_j$. Note that the interaction energy of two spheres is less than that of two points, which follows from Newton's Theorem: for $i \neq j$,

$$\frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} = \int_{\mathbb{R}^3} \Phi_{\delta_{\mathbf{x}_i}}(\mathbf{x}) \delta_{\mathbf{x}_j}(\mathbf{x}) d\mathbf{x} \geq \int_{\mathbb{R}^3} \Phi_{\mu_i}(\mathbf{x}) \delta_{\mathbf{x}_j}(\mathbf{x}) d\mathbf{x} = \int_{\mathbb{R}^3} \Phi_{\delta_{\mathbf{x}_j}}(\mathbf{x}) d\mu_i(\mathbf{x}) d\mathbf{x} \geq 2D(\mu_j, \mu_i)$$

(with equality if the points are far away). Also, for any $j \in \{1, \dots, N\}$ and $k \in \{1, \dots, M\}$,

$$\frac{1}{|\mathbf{x}_j - \mathbf{R}_k|} = \Phi_{\delta_{\mathbf{x}_j}}(\mathbf{R}_k) = \Phi_{\mu_j}(\mathbf{R}_k) = \int_{\mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{R}_k|} d\mu_j(\mathbf{x}).$$

Therefore,

$$\begin{aligned} W_C(\mathbf{x}, \mathbf{R}) &\geq \sum_{i \neq j} D(\mu_i, \mu_j) - \sum_j \sum_k \int_{\mathbb{R}^3} \frac{Z}{|\mathbf{x} - \mathbf{R}_k|} d\mu_j(\mathbf{x}) + \sum_{k < l} \frac{Z^2}{|\mathbf{R}_k - \mathbf{R}_l|} \\ &= D(\mu, \mu) - \int_{\mathbb{R}^3} \Phi(\mathbf{x}) d\mu(\mathbf{x}) + \sum_{k < l} \frac{Z^2}{|\mathbf{R}_k - \mathbf{R}_l|} - \int_{\mathbb{R}^3} \frac{Z}{\text{dist}(\mathbf{x}, \mathbf{R})} d\mu(\mathbf{x}) - \sum_{j=1}^N \frac{1}{d_j}, \end{aligned}$$

where we used that $D(\mu_j, \mu_j) = 1/d_j$ (exercise). For the first three terms we may now use the Basic Electrostatic Inequality, while for the last two we use that

$$\int_{\mathbb{R}^3} \frac{Z}{\text{dist}(\mathbf{x}, \mathbf{R})} d\mu_j(\mathbf{x}) + \frac{1}{d_j} \leq (2Z + 1) \frac{1}{d_j},$$

since for any \mathbf{x} on the support of μ_j and any $k \in \{1, \dots, M\}$

$$|\mathbf{x} - \mathbf{R}_k| \geq |\mathbf{x}_j - \mathbf{R}_k| - |\mathbf{x}_j - \mathbf{x}| \geq d_j - d_j/2 = d_j/2.$$

This finishes the proof of Theorem 7.2.

Exercise 7.1. Prove that (7.8) holds for some $C > 0$. You may also use the identity

$$\int_0^\infty t^{\frac{\alpha}{2}-1} e^{-\pi t |\mathbf{x}-\mathbf{y}|^2} dt = \pi^{-\frac{\alpha}{2}} \Gamma(\frac{\alpha}{2}) |\mathbf{x} - \mathbf{y}|^{-\alpha}, \quad \alpha > 0,$$

to prove that $C = \pi^{-3}$ (for further hints see e.g. [LL01, Chapter 5]).

Exercise 7.2. Compute $D(\mu_j, \mu_j) = 1/d_j$.

7.3. Proof of stability of the second kind. We will now apply the Lieb–Thirring inequality in the simplest available proof of stability for fermions, due to Solovej [Sol06a] (see also [LS10, Section 7.2]), as well as in a straightforward generalization for inverse-square repulsive bosons [LPS15] in three dimensions. We also briefly discuss the situation in lower dimensions.

7.3.1. Fermions. We consider first fermions, possibly with q different species or spin states.

Theorem 7.6 (Stability for fermionic matter). For any number of particles $N, M \geq 1$, for any positions of the nuclei $\mathbf{R} \in \mathbb{R}^{3M}$, and for any mass $m > 0$ and charge $Z > 0$, we have

$$\hat{H}^N(\mathbf{R}) := \sum_{j=1}^N \frac{1}{2m} (-\Delta_{\mathbf{x}_j}) + W_C(\mathbf{x}, \mathbf{R}) \geq -0.62 q^{2/3} m (2Z + 1)^2 (N + M),$$

where the domain of the operator $\hat{H}^N(\mathbf{R})$ is defined w.r.t. q -antisymmetric functions with the form domain $H_{\text{asym}(q)}^1(\mathbb{R}^{3N})$.

Remark 7.7. Note that the result concerns only the symmetry type of one of the species of particles involved (here the electrons), and that the other particles at \mathbf{R}_k may thus be of any type: quantum mechanical bosons, distinguishable particles, or even fixed classical charges. The only property we use for them is their Coulomb interaction and the overall screening among all particles.

Proof. We only need the simpler lower bound given by Baxter's inequality, Theorem 7.2,

$$W_C(\mathbf{x}, \mathbf{R}) \geq -(2Z + 1) \sum_{j=1}^N \frac{1}{\text{dist}(\mathbf{x}_j, \mathbf{R})}.$$

The trick is then just to add and subtract a constant $b > 0$ to the Hamiltonian, writing for simplicity

$$\begin{aligned} \hat{H}^N(\mathbf{R}) &\geq \frac{1}{2m} \sum_{j=1}^N \left[-\Delta_{\mathbf{x}_j} - 2m(2Z + 1) \left(\frac{1}{\text{dist}(\mathbf{x}_j, \mathbf{R})} - b \right) \right] - (2Z + 1)Nb \\ &\geq -\frac{1}{2m} qL_3 (2m(2Z + 1))^{5/2} \int_{\mathbb{R}^3} \left[\frac{1}{\text{dist}(\mathbf{x}, \mathbf{R})} - b \right]_+^{5/2} d\mathbf{x} - (2Z + 1)Nb, \end{aligned}$$

where in the second step we crucially used the q -antisymmetric domain of the operator and the fermionic Lieb–Thirring inequality of Corollary 6.8. Furthermore, using that

$$\left[\frac{1}{\text{dist}(\mathbf{x}, \mathbf{R})} - b \right]_+^{5/2} = \max_{1 \leq k \leq M} \left[\frac{1}{|\mathbf{x} - \mathbf{R}_k|} - b \right]_+^{5/2} \leq \sum_{k=1}^M \left[\frac{1}{|\mathbf{x} - \mathbf{R}_k|} - b \right]_+^{5/2},$$

one may bound

$$\int_{\mathbb{R}^3} \left[\frac{1}{\text{dist}(\mathbf{x}, \mathbf{R})} - b \right]_+^{5/2} d\mathbf{x} \leq M \int_{|\mathbf{x}| \leq 1/b} \left(\frac{1}{|\mathbf{x}|} - b \right)^{5/2} d\mathbf{x} = \frac{5\pi^2}{4} Mb^{-1/2}.$$

Hence,

$$\hat{H}^N(\mathbf{R}) \geq -qL_3 \frac{5\pi^2}{4} (2m)^{3/2} (2Z + 1)^{5/2} Mb^{-1/2} - (2Z + 1)Nb,$$

and after optimizing in $b > 0$,

$$\hat{H}^N(\mathbf{R}) \geq -\frac{3}{2} (5\pi^2 L_3)^{2/3} q^{2/3} m (2Z + 1)^2 M^{2/3} N^{1/3} \geq -0.62 q^{2/3} m (2Z + 1)^2 (N + M),$$

where in the final step we used the best presently known value for L_3 (see Remark 6.2) and Young's inequality (2.4). \square

7.3.2. Inverse-square repulsive bosons. We now consider a system of $N + M$ charged particles, subject to the usual Coulomb interaction W_C , but N of which also experience an additional inverse-square repulsive interaction with coupling parameter β . If we do not impose any symmetry conditions on the particles, the ground state is known to be bosonic. However, thanks to the bosonic Lieb–Thirring inequality of Theorem 6.11, we nevertheless do have stability for $\beta > 0$:

Theorem 7.8 (Stability for inverse-square repulsive bosons). *For any coupling strength $\beta > 0$ there exists a positive constant $C(\beta) = CL_3(\beta)^{2/3} > 0$, such that for any*

number of particles $N, M \geq 1$, for any positions $\mathbf{R} \in \mathbb{R}^{3M}$, and for any mass $m > 0$ and charge $Z > 0$, we have

$$\begin{aligned} \hat{H}_\beta^N(\mathbf{R}) &:= \frac{1}{2m} \left[\sum_{j=1}^N (-\Delta_{\mathbf{x}_j}) + \sum_{1 \leq j < k \leq N} \frac{\beta}{|\mathbf{x}_j - \mathbf{x}_k|^2} \right] + W_C(\mathbf{x}, \mathbf{R}) \\ &\geq -C(\beta) m(2Z + 1)^2(N + M), \end{aligned}$$

where the operator $\hat{H}_\beta^N(\mathbf{R})$ is defined as the Friedrichs extension w.r.t. the form domain $\mathcal{H}_{d=3,N}^1$ in (6.17) (with no symmetry assumptions on the wave functions).

Remark 7.9. We note that since $K_d(\beta) \sim \beta^{2/d}$ or equivalently $L_d(\beta) \sim \beta^{-1}$ as $\beta \rightarrow 0$ for $d \geq 3$ (see Remark 6.13), one has $C(\beta) \sim \beta^{-2/3} \rightarrow \infty$ in the limit of weak interactions. Taking $\beta \sim N^{-1}$ for example corresponds to a **mean-field scaling** of the interaction, and evidently leads to bound similar to $q \sim N$ for fermions, which is too weak for stability. Also note that it may be more natural to incorporate the mass factor $2m$ by rescaling the parameter β .

Proof. We mimic the proof of Theorem 7.6, replacing the fermionic LT with the BLT (6.19) of Theorem 6.11. Thus,

$$\begin{aligned} \hat{H}_\beta^N(\mathbf{R}) &\geq \frac{1}{2m} \left[\hat{T} + \hat{W}_\beta + \hat{V} \right] - (2Z + 1)Nb \\ &\geq -\frac{1}{2m} L_3(\beta) \int_{\mathbb{R}^3} |V_-|^{5/2} - (2Z + 1)Nb, \end{aligned}$$

where

$$V(\mathbf{x}) := -2m(2Z + 1) \left(\frac{1}{\text{dist}(\mathbf{x}, \mathbf{R})} - b \right).$$

The remainder of the proof then goes through exactly as before, with the replacement $qL_3 \rightarrow L_3(\beta)$. \square

7.3.3. Lower dimensions. Consider particles that have been confined to a thin layer, for example by means of a strong transverse external potential, such as

$$V(x, y, z) = V_2(x, y) + C_3|z|^2, \quad C_3 \gg 1.$$

Hence they may effectively only move in the two-dimensional plane $z = 0$, but their interactions could still be the usual Coulomb interactions due to electromagnetism that propagates freely in three dimensions. (If electromagnetism would instead be propagating in only two dimensions, one could argue to instead use the logarithmic 2D analog of the Coulomb potential; see [MS06] for this case.) We may thus keep the interaction term W_C as it is and consider stability under the assumption that all particles are situated in the plane \mathbb{R}^2 :

$$\hat{H}^{N,M} := \sum_{j=1}^N \frac{\hbar^2}{2m_e} (-\Delta_{\mathbf{x}_j}) + \sum_{k=1}^M \frac{\hbar^2}{2m_n} (-\Delta_{\mathbf{R}_k}) + W_C(\mathbf{x}, \mathbf{R}),$$

or, in the case of fixed ‘nuclei’ (or charged impurities in the layer),

$$\hat{H}^N(\mathbf{R}) := \sum_{j=1}^N \frac{\hbar^2}{2m_e} (-\Delta_{\mathbf{x}_j}) + W_C(\mathbf{x}, \mathbf{R}),$$

with $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^{2N}$ and $\mathbf{R} = (\mathbf{R}_1, \dots, \mathbf{R}_M) \in \mathbb{R}^{2M}$.

In this case there are some additional technical complications due to the dimensionality, and one needs to use the positive terms in Baxter's inequality (7.7) as well; see e.g. [LS14, Section 6.2] for details, leading to the following theorem:

Theorem 7.10 (Stability for fermions in 2D). *There exists a constant $C > 0$ such that for any number of particles $N, M \geq 1$, for any positions of the nuclei $\mathbf{R} \in \mathbb{R}^{2M}$, and for any mass $m > 0$ and charge $Z > 0$, we have*

$$\hat{H}^N(\mathbf{R}) := \sum_{j=1}^N \frac{1}{2m} (-\Delta_{\mathbf{x}_j}) + W_C(\mathbf{x}, \mathbf{R}) \geq -C qm(2Z + 1)^2(N + M), \quad (7.10)$$

where the domain of the operator $\hat{H}^N(\mathbf{R})$ is defined w.r.t. q -antisymmetric functions with the form domain $H_{\text{asym}(q)}^1(\mathbb{R}^{2N})$.

Stability has also been extended to anyons in [LS14, Theorem 21] and [LS18], i.e. replacing the fermionic kinetic energy by \hat{T}_α from (3.53), where the resulting difference is just to replace q in the r.h.s. of (7.10) with $1/\alpha_2$ as of Theorem 6.14. In other words, one has stability for any type of (ideal) anyons except for bosons for which $\alpha_2 = \alpha = 0$.

Theorem 7.11 (Stability for anyons in 2D). *There exists a constant $C > 0$ such that for any number of particles $N, M \geq 1$, for any positions of nuclei $\mathbf{R} \in \mathbb{R}^{2M}$, and for any mass $m > 0$ and charge $Z > 0$, and statistics parameter $\alpha \in \mathbb{R}$, we have*

$$\hat{H}_\alpha^N(\mathbf{R}) := \frac{1}{2m} \hat{T}_\alpha + W_C(\mathbf{x}, \mathbf{R}) \geq -C \alpha_2^{-1} m(2Z + 1)^2(N + M),$$

where the N -anyon kinetic energy \hat{T}_α is defined as the Friedrichs extension w.r.t. functions $C_c^\infty(\mathbb{R}^{2N} \setminus \Delta) \cap L_{\text{sym}}^2(\mathbb{R}^{2N})$.

For bosons in two dimensions with inverse-square repulsion one may proceed in the same way and use the BLT of Theorem 6.11 to prove stability for any fixed coupling $\beta > 0$. However the bound diverges as $\beta \rightarrow 0$ since $K_2(\beta) \rightarrow 0$ implies $L_2(\beta) \rightarrow +\infty$.

In one dimension we have, as previously discussed, a correspondence between fermions and bosons in the form domain $H_0^1(\mathbb{R}^N \setminus \Delta)$. Therefore any repulsive interaction which forces such a hard-core vanishing condition will be at least as strong as for non-interacting fermions. Note also that the Hardy inequality of Theorem 4.11 is then available, so that we get an inverse-square repulsion for free. Unfortunately, however, the attractive 3D Coulomb potential $-|\mathbf{x}|^{-1}$ is too singular in one dimension to ensure stability even for a single ‘‘atom’’.

Exercise 7.3. *Fill in the details above to prove stability for fermions in 2D.*

Exercise 7.4. *What is the situation concerning stability in 1D if one puts a hard-core vanishing condition for the electrons at each of the nuclei?*

7.4. Instability of matter. We have seen that bulk matter in 3D consisting to at least one part (a nonvanishing fraction) of fermions is stable, and that stability also holds if the particles are bosons with an additional inverse-square repulsion. However, switching off this repulsion with $\beta \rightarrow 0$ according to Remark 7.9, or relaxing the Pauli principle to allow for arbitrarily many particles $q = N \rightarrow \infty$ in each one-body state, seems to lead to **instability**, and indeed this may be shown to be the correct conclusion.

7.4.1. *Instability for charged bosons.* We define two purely bosonic ground-state energies for N electrons and M nuclei; one with the nuclei being fixed, classical particles but at their worst possible positions,

$$E_0(N, M) := \inf_{\mathbf{R} \in \mathbb{R}^{3M}} \inf \sigma(\hat{H}^N(\mathbf{R})|_{\mathcal{H}^N}),$$

and one where they are true quantum particles with a finite mass $m_n > 0$,

$$\tilde{E}_0(N, M) := \inf \sigma(\hat{H}^{N,M}|_{\mathcal{H}^{N,M}}).$$

In the first case, which was settled early on by [LD68] (lower bound) and [Lie79] (upper bound), one has the following instability result, matching the lower bound of Theorem 7.6 with $q = N$:

Theorem 7.12 (Instability for bosons with fixed nuclei). *There exist constants $C_- > C_+ > 0$ (depending on m_e, m_n, Z and κ) such that for any $N, M \in \mathbb{N}$ particles, $N/M = \kappa$,*

$$-C_- N^{5/3} < E_0(N, M) < -C_+ N^{5/3}.$$

However, in the case of the second definition of energy \tilde{E}_0 , it is potentially increased and thus less divergent due to the uncertainty principle for the quantum nuclei — and indeed this was shown to be the case — although not sufficiently so to make the system thermodynamically stable. The result is given in the following theorem which was worked out in several steps and over many years [Dys67, CLY88, LS04, Sol06b]:

Theorem 7.13 (Instability for bosons with moving nuclei). *Let $Z = 1$ and $m_e = m_n = 1$. There exists a constant $C > 0$ such that*

$$\min_{N+M=K} \tilde{E}_0(N, M) = -CK^{7/5} + o(K^{7/5}), \quad \text{as } K \rightarrow \infty.$$

In fact,

$$-C = \inf \left\{ \int_{\mathbb{R}^3} |\nabla \Phi|^2 - I_0 \int_{\mathbb{R}^3} \Phi^{5/2} : \Phi \in H^1(\mathbb{R}^3; \mathbb{R}_+), \int_{\mathbb{R}^3} \Phi^2 = 1 \right\},$$

where (Foldy's constant)

$$I_0 = \frac{2 \Gamma(3/4)}{5 \Gamma(5/4)} \left(\frac{2}{\pi} \right)^{1/4}.$$

We refer to [LS10, LSSY05] for pedagogically outlined proofs of these results and for further discussions on instability. For completeness we provide only the following simpler version of instability with fixed nuclei, from [Lie79] and [LS10, Proposition 7.1].

Theorem 7.14. *Assume that $N = ZM$, $Z > 0$, $M = n^3$, $n \in \mathbb{N}$. Then there exists a normalized bosonic N -body state $\Psi \in L^2_{\text{sym}}((\mathbb{R}^3)^N)$ and positions $\mathbf{R} = (\mathbf{R}_1, \dots, \mathbf{R}_M) \in \mathbb{R}^{3M}$, such that*

$$\langle \Psi, \hat{H}^N(\mathbf{R}) \Psi \rangle \leq -CZ^{4/3} N^{5/3},$$

for a constant $C > 0$ independent of N, Z, M .

Proof. Let $\Psi(\mathbf{x}) = \prod_{j=1}^N \phi_\lambda(\mathbf{x}_j)$, with $\phi_\lambda(\mathbf{x}) = \lambda^{3/2} \phi(\lambda \mathbf{x})$, $\lambda > 0$, such that $\phi \in C_c^\infty(\mathbb{R}^3)$ and $\int |\phi_\lambda|^2 = \int |\phi|^2 = 1$. Then

$$\begin{aligned} \langle \Psi, \hat{H}^N(\mathbf{R}) \Psi \rangle &= N \int_{\mathbb{R}^3} |\nabla \phi_\lambda|^2 + \frac{1}{2} N(N-1) \int_{\mathbb{R}^6} \frac{|\phi_\lambda(\mathbf{x})|^2 |\phi_\lambda(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y} \\ &\quad - ZN \sum_{k=1}^M \int_{\mathbb{R}^3} \frac{|\phi_\lambda(\mathbf{x})|^2}{|\mathbf{x} - \mathbf{R}_k|} d\mathbf{x} + Z^2 \sum_{k < l} \frac{1}{|\mathbf{R}_k - \mathbf{R}_l|} \\ &= N\lambda^2 \int |\nabla \phi|^2 + \lambda W[\phi, \lambda \mathbf{R}], \end{aligned}$$

where

$$\begin{aligned} W[\phi, \mathbf{R}] &:= \frac{1}{2} N(N-1) \int_{\mathbb{R}^6} \frac{|\phi(\mathbf{x})|^2 |\phi(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y} \\ &\quad - ZN \sum_{k=1}^M \int_{\mathbb{R}^3} \frac{|\phi(\mathbf{x})|^2}{|\mathbf{x} - \mathbf{R}_k|} d\mathbf{x} + Z^2 \sum_{k < l} \frac{1}{|\mathbf{R}_k - \mathbf{R}_l|}. \end{aligned}$$

We claim that we can find ϕ and positions \mathbf{R} such that

$$W[\phi, \mathbf{R}] \leq -C Z^{2/3} N^{4/3}$$

for some $C > 0$. This will then prove the theorem by the choice of the optimal

$$\lambda = \frac{1}{2} N^{1/3} Z^{2/3} \frac{C}{\int_{\mathbb{R}^3} |\nabla \phi|^2},$$

so that

$$\langle \Psi, \hat{H}^N(\mathbf{R}) \Psi \rangle \leq -\frac{1}{4} \frac{C^2}{\int_{\mathbb{R}^3} |\nabla \phi|^2} Z^{4/3} N^{5/3}.$$

To prove the above claim, we consider a partition of the support of ϕ into cells Γ_k , $k = 1, \dots, M$, such that

$$\int_{\Gamma_k} |\phi(\mathbf{x})|^2 d\mathbf{x} = \frac{1}{M}$$

and place each nucleus $\mathbf{R}_k \in \Gamma_k$. In order to estimate the corresponding energy we perform a clever averaging trick, namely consider averaging the positions \mathbf{R}_k subject to the probability distribution $\mu_k := M |\phi|_{\Gamma_k}|^2$, that is

$$\langle W[\phi, \mathbf{R}] \rangle_{\mathbf{R}_k} := \int_{\Gamma_k} W[\phi, \mathbf{R}] M |\phi(\mathbf{R}_k)|^2 d\mathbf{R}_k.$$

Applying this averaging over every k to the terms in $W[\phi, \mathbf{R}]$, we find:

- The electron-electron repulsion term is unchanged.
- For the electron-nucleus interaction term,

$$\sum_{k=1}^M ZM \int_{\Gamma_k} \int_{\mathbb{R}^3} \frac{|\phi(\mathbf{x})|^2}{|\mathbf{x} - \mathbf{R}_k|} |\phi(\mathbf{R}_k)|^2 d\mathbf{R}_k = ZM \int_{\mathbb{R}^6} \frac{|\phi(\mathbf{x})|^2 |\phi(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y}.$$

- For the nucleus-nucleus repulsion term,

$$\begin{aligned} & \sum_{k < l}^M Z^2 M^2 \int_{\Gamma_k} \int_{\Gamma_l} \frac{|\phi(\mathbf{R}_k)|^2 |\phi(\mathbf{R}_l)|^2}{|\mathbf{R}_k - \mathbf{R}_l|} d\mathbf{R}_k d\mathbf{R}_l \\ &= \frac{1}{2} Z^2 M^2 \int_{\mathbb{R}^6} \frac{|\phi(\mathbf{x})|^2 |\phi(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y} - \sum_{k=1}^M Z^2 M^2 \int_{\Gamma_k \times \Gamma_k} \frac{|\phi(\mathbf{x})|^2 |\phi(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y}. \end{aligned}$$

Hence, in the average $\langle W[\phi, \mathbf{R}] \rangle_{\mathbf{R}} = \langle W[\phi, \mathbf{R}] \rangle_{\mathbf{R}_1, \dots, \mathbf{R}_k}$ there are three terms involving the same \mathbb{R}^6 integral, with the overall coefficient

$$\frac{1}{2} N(N-1) - ZNM + \frac{1}{2} Z^2 M^2 = -\frac{1}{2} N \leq 0,$$

so that

$$\inf_{\mathbf{R}_k \in \Gamma_k} W[\phi, \mathbf{R}] \leq \langle W[\phi, \mathbf{R}] \rangle_{\mathbf{R}} \leq -Z^2 M^2 \sum_{k=1}^M \int_{\Gamma_k \times \Gamma_k} \frac{|\phi(\mathbf{x})|^2 |\phi(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y}.$$

It thus remains to estimate the Coulomb self-energy of the normalized measures μ_k ,

$$2D(\mu_k, \mu_k) = \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{y}|} d\mu_k(\mathbf{x}) d\mu_k(\mathbf{y}) \geq \int_{\partial B_k \times \partial B_k} \frac{1}{|\mathbf{x} - \mathbf{y}|} d\sigma(\mathbf{x}) d\sigma(\mathbf{y}) = \frac{1}{r_k},$$

where we used that the self-energy of μ_k is bounded below by the infimum over all probability measures over the smallest ball B_k which contains Γ_k , of radius $r_k > 0$. The minimal such distribution on B_k is given by the uniform measure σ over the boundary ∂B_k (consider averaging over rotations and Newton's theorem, as well as Exercise 7.2; the issue is discussed in detail in [LL01, Section 11.15]). Hence,

$$\sum_k 2D(\mu_k, \mu_k) \geq \sum_{k=1}^M \frac{1}{r_k} \geq M \frac{1}{\frac{1}{M} \sum_{k=1}^M r_k},$$

by convexity of the map $0 < x \mapsto x^{-1}$.

Finally, we prove that by an appropriate choice of ϕ ,

$$\frac{1}{M} \sum_{k=1}^M r_k \leq \frac{3}{2} M^{-1/3}, \quad (7.11)$$

so that

$$\inf_{\mathbf{R}_k \in \Gamma_k} W[\phi, \mathbf{R}] \leq -Z^2 \sum_k \frac{1}{r_k} \leq -\frac{2}{3} Z^2 M^{4/3} = -\frac{2}{3} Z^{2/3} N^{4/3}.$$

Namely, we may take $f \in C_c^\infty([0, 1]; \mathbb{R}_+)$ and

$$\phi(x, y, z) = f(x)f(y)f(z),$$

and further divide the unit interval into n sub-intervals I_p s.t.

$$\int_{I_p} |f(x)|^2 dx = \frac{1}{n}, \quad p = 1, \dots, n.$$

This produces $M = n^3$ cells of the form

$$\Gamma_k = I_{p_1} \times I_{p_2} \times I_{p_3}, \quad p_j \in \{1, \dots, n\},$$

with the radius of the smallest enclosing ball

$$r_k = \frac{1}{2} (|I_{p_1}|^2 + |I_{p_2}|^2 + |I_{p_3}|^2)^{1/2} \leq \frac{1}{2} (|I_{p_1}| + |I_{p_2}| + |I_{p_3}|).$$

Thus, by symmetry,

$$\sum_{k=1}^{n^3} r_k \leq \frac{3}{2} \sum_k |I_{p_1}| = \frac{3}{2} n^2,$$

which proves (7.11) and hence the claim and therefore the theorem. \square

7.4.2. Instability for attractive interactions. If the interactions within a species of particle, which above were repulsive Coulomb interactions or possibly inverse-square repulsion, are replaced by *attractive* interactions, then stability no longer holds, even for fermions. The following theorem is taken from [Sol12, Theorem 3.6].

Theorem 7.15 (Fermionic instability for attractive 2-body potentials). *Assume that the two-body potential $W: \mathbb{R}^d \rightarrow \mathbb{R}$ satisfies $W(\mathbf{r}) \leq -c < 0$ for all \mathbf{r} in some ball around the origin, and consider the N -body operator*

$$\hat{H}_N = \hat{T} + \hat{W} = \frac{1}{2m} \sum_{j=1}^N (-\Delta_{\mathbf{x}_j}) + \sum_{1 \leq i < j \leq N} W(\mathbf{x}_i - \mathbf{x}_j),$$

acting in $L^2_{\text{asym}}((\mathbb{R}^d)^N) = \bigwedge^N L^2(\mathbb{R}^d)$. If $d \geq 3$ then \hat{H}_N cannot be stable of the second kind, i.e. we can find a sequence of normalized vectors $\Psi_N \in L^2_{\text{asym}}(\mathbb{R}^{dN})$ in the form domain of \hat{H}_N such that

$$\lim_{N \rightarrow \infty} N^{-1} \langle \Psi_N, \hat{H}_N \Psi_N \rangle = -\infty.$$

Proof. Assume that $W(\mathbf{r}) \leq -c < 0$ on the ball $B_R(\mathbf{0})$, $R > 0$. Consider a fermionic N -body state $\Psi_N \in \bigwedge^N L^2_c(B_R(\mathbf{0}))$, $\|\Psi_N\|_{L^2} = 1$, with a kinetic energy

$$\langle \Psi_N, \hat{T} \Psi_N \rangle \leq C_d N^{1+2/d} R^{-2},$$

for some constant $C_d > 0$ (indeed this was done in Exercise 5.3, modulo a trivial geometric equivalence). Thus

$$N^{-1} \langle \Psi_N, \hat{H}_N \Psi_N \rangle \leq C_d N^{2/d} R^{-2} - \frac{1}{2} (N-1)c,$$

so that instability occurs when $d \geq 3$. \square

7.5. Extensivity of matter. Finally, we have the following formulation of the extensivity of fermionic matter, adopted from [Thi02, Theorem 4.3.3] and [LS10], and extended here also to arbitrary dimensions and to inverse-square repulsive bosons (as well as to any other operators of similar scaling for which a kinetic-exclusion energy inequality holds):

Theorem 7.16 (Extensivity of the volume). *Consider on \mathbb{R}^d the N -body operators*

$$\hat{H} := \hat{T}|_{\mathcal{H}_{\text{asym}(q)}} + \hat{V}_R \quad \text{or} \quad \hat{H} := \hat{T} + \hat{W}_\beta + \hat{V}_R, \quad \beta > 0,$$

and where \hat{V}_R with the parameter R is an operator assumed to scale with the inverse length, such as the Coulomb interaction $\hat{V}_R = W_C(\cdot, R)$ with some fixed set of nuclei R . Assume that it admits stability of the second kind, $\hat{H} \geq -AN$, for some $A > 0$ independent of R

and N . Then, given any $B \geq 0$, there exists a constant $C_d > 0$ such that for any state $\Psi \in \mathcal{Q}(\hat{H})$ with low energy in the sense that $-AN \leq \langle \hat{H} \rangle_\Psi \leq BN$, in this state

$$\left(\frac{|\Omega|}{N}\right)^{\frac{2}{2+d}} \geq C_d \frac{\int_\Omega \varrho_\Psi}{N},$$

for any $\Omega \subseteq \mathbb{R}^d$. That is, any volume which contains a non-vanishing fraction of the particles cannot be smaller than a corresponding non-vanishing fraction of N .

Proof. We have for any L^2 -normalized Ψ , by the kinetic-exclusion inequality (LT/BLT),

$$T[\Psi] + W_\beta[\Psi] \geq K_d(\beta) \int_{\mathbb{R}^d} \varrho_\Psi^{1+2/d}, \quad (7.12)$$

and by stability, for any R ,

$$T[\Psi] + W_\beta[\Psi] + V_R[\Psi] = \langle \hat{H} \rangle_\Psi \geq -AN. \quad (7.13)$$

Consider $\Psi_\lambda(\mathbf{x}) = \lambda^{dN/2} \Psi(\lambda \mathbf{x})$, $\lambda \in (0, 1)$, and employ the scaling properties of \hat{T} , \hat{W}_β and \hat{V}_R :

$$T[\Psi_\lambda] + W_\beta[\Psi_\lambda] + V_{\lambda^{-1}R}[\Psi_\lambda] = \lambda^2 T[\Psi] + \lambda^2 W_\beta[\Psi] + \lambda V_R[\Psi].$$

Therefore, by (7.13),

$$\lambda(T[\Psi] + W_\beta[\Psi]) + V_R[\Psi] \geq -AN/\lambda \quad (7.14)$$

(equivalently, this is the statement that in a Coulomb system the energy scales linearly with the mass, as we can also see explicitly in our bounds concerning stability).

Let us fix Ψ with energy $E := \langle \hat{H} \rangle_\Psi \geq -AN$ and also assume that $E \leq BN$. From (7.14),

$$E = (1 - \lambda)(T[\Psi] + W_\beta[\Psi]) + \lambda(T[\Psi] + W_\beta[\Psi]) + V_R[\Psi] \geq (1 - \lambda)(T[\Psi] + W_\beta[\Psi]) - AN/\lambda,$$

thus

$$T[\Psi] + W_\beta[\Psi] \leq \frac{E}{1 - \lambda} + \frac{AN}{\lambda(1 - \lambda)} = \frac{E + AN}{1 - \lambda} + \frac{AN}{\lambda}.$$

We are here free to choose $\lambda \in (0, 1)$, and the optimal choice

$$\lambda = \frac{\sqrt{AN}}{\sqrt{AN} + \sqrt{E + AN}}$$

produces the bound

$$T[\Psi] + W_\beta[\Psi] \leq \left(\sqrt{AN} + \sqrt{E + AN}\right)^2 \leq N \left(\sqrt{A} + \sqrt{A + B}\right)^2,$$

that is the kinetic-exclusion energy in such a state is at most $O(N)$. For any $\Omega \subseteq \mathbb{R}^d$ we then obtain, using Hölder and (7.12),

$$\begin{aligned} \int_\Omega \varrho_\Psi &\leq \left(\int_\Omega \varrho_\Psi^{1+2/d}\right)^{\frac{d}{2+d}} \left(\int_\Omega 1\right)^{\frac{2}{2+d}} \leq \left(K_d(\beta)^{-1} N \left(\sqrt{A} + \sqrt{A + B}\right)^2\right)^{\frac{d}{2+d}} |\Omega|^{\frac{2}{2+d}} \\ &= C_d^{-1} N (|\Omega|/N)^{\frac{2}{2+d}}, \end{aligned}$$

with $C_d > 0$ for fixed $\beta > 0$, for the expected number of particles on Ω . \square

The above theorem then explains why fermionic matter occupies a volume that grows at least linearly with the number of particles. This concerns the ground state or a not too excited state, namely note that the upper bound BN on its energy was required since we may of course compress lots of particles to a small volume away from the nuclei R , with a high cost in energy. For simplicity we could have also taken $B = 0$ in the above theorem. See [LS10, Theorem 7.2] for other formulations of extensivity for fermions.

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