Mathematical Quantum Mechanics with Applications

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Abstract

In these notes, we introduce basic mathematical tools needed for the rigorous analysis of quantum systems and we present some applications in many body quantum mechanics. The first part focuses on the spectral theorem for self-adjoint operators and discusses several of its applications. In the second part we study low-energy properties of bosonic many body systems consisting of N particles moving in $\mathbb{R}^3$ and interacting through a two-body potential. Such systems may exhibit the phenomenon of Bose-Einstein Condensation which is explained in detail in the so called mean field regime. The notes conclude with basic results on the Bose gas in the more challenging Gross-Pitaevskii and thermodynamic limits.

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1 Introduction

Consider a system of N identical, non-relativistic, spinless quantum particles moving in a box $\Lambda_L \subset \mathbb{R}^3$ of side length L. Such a system is mathematically described by a normalized wave function $\psi_N \in L^2(\Lambda_L^N)$ with the interpretation that

$$d\mu_{\psi_N}(x_1, \ldots, x_N) = |\psi_N(x_1, \ldots, x_N)|^2 \, dx_1 \ldots dx_N$$

defines the probability of finding the N particles near $(x_1, \ldots, x_N) \in \Lambda_L^N$. In this course, we restrict our attention to bosons which are particles that obey the so called Bose-Einstein statistics. Bosons are described by wave functions $\psi_N \in L_s^2(\Lambda_L^N)$ which are symmetric under particle exchange, meaning that

$$\psi_N(x_1, x_2, \ldots, x_N) = \psi_N\big(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(N)}\big)$$

for *a.e.* $(x_1, x_2, \ldots, x_N) \in \Lambda_L^N$ and for all permutations $\sigma \in \mathfrak{S}_N$ of N elements. In particular, each of the N particles can occupy the same one particle wave function $\varphi \in L^2(\Lambda)$ such that, for instance, $\varphi^{\otimes N} \in L_s^2(\Lambda_L^N)$ is a bosonic wave function. Bosons are of particular interest in physics, because at low temperature they undergo a phase transition to form a Bose-Einstein condensate. The discovery of BEC goes back to N. Bose and A. Einstein [10, 21, 22]. Its experimental verification for strongly dilute systems [1, 20] was awarded in the late nineties with the Nobel prize in physics.

In a Bose-Einstein condensate, the majority of the $N \gg 1$ particles behaves like a single one body wave function $\varphi \in L^2(\Lambda_L)$, the condensate. Mathematically, this means that ψ_N is close to a tensor product $\varphi^{\otimes N}$, in a suitable sense. This provides a very simple description of the large many body system in terms of an effective one body system. In particular, physical observables are essentially determined by the condensate state φ.

In quantum mechanics, physical observables are described by self-adjoint operators $A : D(A) \to L^2(\Lambda_L^N)$. Given such an observable, its expectation value with regards to the state $\psi_N \in L_s^2(\Lambda_L^N)$ equals the inner product $\langle \psi_N, A\psi_N \rangle$. For example, the multiplication operator $\widehat{x}_i$ that multiplies ψ_N by $x_i \in \Lambda_L$ measures the particle position of particle i (and thus, by Bose-Einstein symmetry, the position of any one, fixed particle). With the probabilistic interpretation of $|\psi_N(x)|^2 \, dx_1 \ldots dx_N$, notice that

$$\langle \psi_N, \widehat{x}_i \, \psi_N \rangle = \int_{\lambda_L} x_i \, |\psi_N(x_1, \ldots, x_N)|^2 \, dx_1 \ldots dx_N$$

corresponds to a probabilistic average. Analogously, $\langle \psi_N, A\psi_N \rangle$ for general self-adjoint $A : D(A) \to L^2(\Lambda_L^N)$ has a probabilistic interpretation, based on the spectral theorem for self-adjoint operators which tells us that A can be diagonalized in a suitable sense.

A particularly important observable in physics is the energy of the system. In case of a non-interacting gas of N particles without the presence of external fields, the energy is purely kinetic and H_N takes the form

$$H_N^{\text{free}} = \sum_{i=1}^{N} (-\Delta_{x_i}),$$

where Δ_{x_i} denotes the Laplacian w.r.t. $x_i \in \Lambda_L$, describing the kinetic energy of the i-th particle. For simplicity, let us impose periodic boundary conditions s.t. a complete orthonormal set of eigenfunctions of H_N is given by N-fold symmetric tensor products of the plane waves $\Lambda_L \ni x \mapsto \varphi_p(x) = |\Lambda_L|^{-3/2} e^{ipx} \in L^2(\Lambda_L)$, where $p \in \frac{2\pi}{L}\mathbb{Z}^3$. A plane wave φ_p describes in quantum mechanics a particle with momentum p (the possible momenta are discrete, in contrast to a classically mechanical description). The eigenvalues of H_N are consequently given by finite sums of the form

$$\sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3} n_p p^2 \qquad \text{with the restriction that} \qquad \sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3} n_p = N.$$

For this explicitly solvable system, notice that the ground state wave function ψ_N, the eigenfunction corresponding to the lowest possible energy $E_N = 0$, equals indeed the tensor product $\psi_N = \varphi_0^{\otimes N}$: in the ground state, the non-interacting system of bosons exhibits Bose-Einstein condensation into the constant wave function φ_0.

Despite typical experiments analyzing strongly dilute gas samples, a realistic description should take into account interactions between the particles. Considering only pair interactions for simplicity, this can be modeled through Hamiltonians of the form

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i}) + \sum_{1\leq i<j\leq N} v(x_i - x_j).$$

In this case, H_N can not be diagonalized explicitly anymore. Can we still determine the ground state energy and higher eigenvalues? Up to which degree of accuracy? And does the ground state exhibit Bose-Einstein condensation in dilute regimes, for instance in regimes of small number of particles density $\rho = N/L^3 \ll 1$?

Motivated by the preceding discussion, the aim of these notes is twofold: first, we introduce the functional analytic tools that are needed to describe and analyze quantum mechanical systems. Most importantly, this includes a thorough discussion of the spectral theorem for general self-adjoint operators in Hilbert spaces and several of its applications. In the second part, we then study weakly interacting Bose gases and understand whether they exhibit Bose-Einstein condensation. Here, we start with the simplest, non-trivial interacting systems called mean field systems. In such a regime, systems of N bosons trapped in a region of $\mathbb{R}^3$ are described by Hamiltonians

$$H_N^{mf} = \sum_{i=1}^{N} \big(-\Delta_{x_i} + V_{\text{ext}}(x_i) \big) + \frac{1}{N} \sum_{1\leq i<j\leq N} v(x_i - x_j),$$

where the factor N^{-1} in front of the two-body interaction ensures that the kinetic and potential energies are of the same order in N. Among other results, we will show that, in the limit of large N, the ground state of the system exhibits Bose-Einstein condensation into the minimizer of the non-linear Hartree energy functional

$$\mathcal{E}_{\text{H}}(\varphi) = \int \Big(|\nabla\varphi|^2 + V_{\text{ext}}|\varphi|^2 + \frac{1}{2}\big(v * |\varphi|^2\big)|\varphi|^2 \Big),$$

which solves, for suitable $\varepsilon \in \mathbb{R}$, the non-linear Hartree equation

$$-\Delta\varphi + V_{\text{ext}}\varphi + \big(v * |\varphi|^2\big)\varphi = \varepsilon\varphi.$$

The mean field scaling describes a situation in which every particle interacts equally strongly with all of the other particles so that, effectively, the potential that is experienced by a fixed particle is given by an average field generated by the remaining particles.

After discussing mean field systems, the last part discusses basic results in the more challenging Gross-Pitaevskii and thermodynamic limits, placing N particles in a box $[-\frac{L}{2}, \frac{L}{2}]^3$ of sidelength L and studying the corresponding ground state energy in the limit $N, L \to \infty$ such that the particle density $\rho = \frac{N}{L^3}$ either tends to zero (ultra-dilute scaling limits) or is fixed, but small. The so called Gross-Pitaevskii scaling corresponds to the choice $L = N$ and corresponds to the simplest, non-trivial ultra-dilute scaling limit. The infinite number of particles and infinite volume limit in which the density ρ remains fixed corresponds to the thermodynamic limit.

2 Selected Topics in Functional Analysis

In this section we introduce several important tools for the rigorous analysis of quantum systems. The presentation mostly follows [55, 56, 57, 58].

2.1 Hilbert Spaces

Systems in quantum mechanics are described with the help of complex Hilbert spaces: let $\mathcal{H}$ be a vector space over $\mathbb{C}$. Recall that $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ is an *inner or scalar product* if it satisfies

i) for all $\psi \in \mathcal{H}$, the map $\mathcal{H} \ni \varphi \mapsto \langle \psi, \varphi \rangle \in \mathbb{C}$ is linear,

ii) for all $\psi, \varphi \in \mathcal{H}$, we have $\langle \psi, \varphi \rangle = \overline{\langle \varphi, \psi \rangle}$,

iii) for all $\psi \in \mathcal{H}$, we have that $\langle \psi, \psi \rangle \geq 0$ with $\langle \psi, \psi \rangle = 0$ if and only if $\psi = 0 \in \mathcal{H}$.

An inner product induces a norm, defined via $\| \cdot \| = \sqrt{\langle \cdot, \cdot \rangle}$. A complex Hilbert space is a pair $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ of a complex linear space with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ s.t. $\mathcal{H}$ is complete w.r.t. the norm induced by $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. Two vectors ψ, φ are called orthogonal if $\langle \psi, \varphi \rangle = 0$. Given a set $M \subset \mathcal{H}$, its orthogonal complement $M^\perp$ is defined as

$$M^\perp = \{\psi \in \mathcal{H} : \langle \psi, \varphi \rangle = 0 \; \forall \varphi \in M\}.$$

It holds true that $\mathcal{H} = M \oplus M^\perp$, s.t. $M \cap M^\perp = \{0\}$, for any closed subspace $M \subset \mathcal{H}$. An orthonormal set is a set of normalized vectors in which each two non-equal elements are orthogonal to each other. An orthonormal basis $S \subset \mathcal{H}$ is an orthonormal set for which there does not exist another orthonormal set which contains S as a proper subset. Every Hilbert space has an orthonormal basis. Unless stated otherwise, we work for simplicity with separable Hilbert spaces, which are spaces that contain a countable, dense subset and hence, by Gram-Schmidt, a countable orthonormal basis.

Problem 2.1. *Prove that an orthonormal sequence $(\psi_j)_{j \in \mathbb{N}}$ is an orthonormal basis in $\mathcal{H}$ if and only if every vector $\psi \in \mathcal{H}$ has the representation $\psi = \sum_{j \in \mathbb{N}} \langle \psi_j, \psi \rangle \psi_j$.*

Example 2.1 (L^2*-spaces*)**.** *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space. Then the set of equivalence classes $L^2(\Omega, \mathcal{A}, \mu) = \{f : \Omega \to \mathbb{C}$ measurable s.t. $\int_\Omega |f|^2 \, d\mu < \infty\}$, equipped with the usual addition and scalar multiplication and the inner product*

$$\langle f, g \rangle_2 = \int_\Omega \overline{f} g \, d\mu$$

defines a complex Hilbert space.

Example 2.2 (Sobolev spaces)**.** *Let $\Omega \subset \mathbb{R}^d$ be open, then*

$$H^1(\Omega) = \Big\{ \psi \in L^2(\Omega) = L^2(\Omega, \mathcal{M}_{\lambda_d^*}, \lambda_d) : \partial_i \psi \in L^2(\Omega), \forall i = 1, \dots, d \Big\},$$

is a Hilbert space when equipped with

$$\langle \psi, \varphi \rangle_{H^1} = \int_\Omega dx\, \overline{\psi}(x)\varphi(x) + \int_\Omega dx\, \nabla\overline{\varphi}(x) \cdot \nabla\psi(x).$$

Here, $\partial_i \psi$ denotes the i-th distributional derivative of ψ and $\nabla = (\partial_1, \ldots, \partial_d)$.

In quantum mechanics, the space $L^2(\Omega, \mathcal{M}_{\lambda_d^*}, \lambda_d) = L^2(\Omega)$ (where $\mathcal{M}_{\lambda_d^*}$ denotes the Lebesgue σ-algebra induced by the d-dimensional outer Lebesgue measure and λ_d denotes the d-dimensional Lebesgue measure) is used to describe a particle in $\Omega \subset \mathbb{R}^d$. The state of the system is described by a normalized vector, called wave function, $\psi \in L^2(\Omega)$. The interpretation is that $d\mu_\psi(x_1, \ldots, x_d) = |\psi(x_1, \ldots, x_d)|^2\ dx_1 \ldots dx_d$ measures the probability for finding the particle in a particular region in $\Omega \subset \mathbb{R}^d$.

To describe many particle systems in quantum mechanics, one uses the tensor product of Hilbert spaces. Given two Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$ and vectors $\psi_1 \in \mathcal{H}_1, \psi_2 \in \mathcal{H}_2$ we denote by $\psi_1 \otimes \psi_2 : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathbb{C}$ the conjugate bilinear form, defined by

$$(\psi_1 \otimes \psi_2)(\varphi_1, \varphi_2) = \langle \varphi_1, \psi_1 \rangle_{\mathcal{H}_1} \langle \varphi_2, \psi_2 \rangle_{\mathcal{H}_2}$$

For such forms, we define

$$\langle \psi_1 \otimes \psi_2, \xi_1 \otimes \xi_2 \rangle_{\mathcal{H}_1 \otimes \mathcal{H}_2} = \langle \psi_1, \xi_1 \rangle_{\mathcal{H}_1} \langle \psi_2, \xi_2 \rangle_{\mathcal{H}_2}.$$

By linearity we can extend this map to the linear space $\mathcal{E}$ of finite linear combinations of the maps $\psi_1 \otimes \psi_2 : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathbb{C}$, $\psi_1 \in \mathcal{H}_1, \psi_2 \in \mathcal{H}_2$, and this yields an inner product.

The tensor product Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ of $\mathcal{H}_1$ and $\mathcal{H}_2$ is defined as the completion of the the linear space $\mathcal{E}$ w.r.t. the norm induced by $\langle \cdot, \cdot \rangle_{\mathcal{H}_1 \otimes \mathcal{H}_2}$.

Lemma 2.1. *If $(\psi_\alpha)_{\alpha\in\mathbb{N}}$ and $(\varphi_\beta)_{\beta\in\mathbb{N}}$ are orthonormal bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, then $(\psi_\alpha \otimes \varphi_\beta)_{(\alpha,\beta)\in\mathbb{N}\times\mathbb{N}}$ is an orthonormal basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$.*

Proof. The sequence $(\psi_\alpha \otimes \varphi_\beta)_{(\alpha,\beta)\in\mathbb{N}\times\mathbb{N}}$ is an orthonormal sequence and the claim follows if we can prove that $\mathcal{E}$ is contained in $\mathcal{S} = \overline{\text{span}(\psi_\alpha \otimes \varphi_\beta : \alpha, \beta \in \mathbb{N})}$ (why?). To this end, it is enough to show that $\zeta \otimes \xi \in \mathcal{S}$ for every $\zeta \in \mathcal{H}_1, \xi \in \mathcal{H}_2$. By assumption on $(\psi_\alpha)_{\alpha\in\mathbb{N}}$ and $(\varphi_\beta)_{\beta\in\mathbb{N}}$, we can write

$$\zeta = \sum_{\alpha\in\mathbb{N}} c_\alpha \psi_\alpha, \quad \xi = \sum_{\beta\in\mathbb{N}} d_\beta \varphi_\beta$$

with

$$\|\zeta\|^2_{\mathcal{H}_1} = \sum_{\alpha\in\mathbb{N}} |c_\alpha|^2, \quad \|\xi\|^2_{\mathcal{H}_2} = \sum_{\beta\in\mathbb{N}} |d_\beta|^2.$$

This implies $\sum_{\alpha,\beta\in\mathbb{N}} |c_\alpha d_\beta|^2 < \infty$ which means that $\sum_{\alpha,\beta\in\mathbb{N}} c_\alpha d_\beta \varphi_\alpha \otimes \psi_\beta \in \mathcal{S}$. Finally, approximating $\zeta\otimes\xi$ by $\sum_{\alpha,\beta\in\mathbb{N}:\alpha,\beta\le N} c_\alpha d_\beta \varphi_\alpha\otimes\psi_\beta$, we find that

$$\begin{aligned}
&\limsup_{N\to\infty}\Big\|\zeta\otimes\xi-\sum_{\alpha,\beta\in\mathbb{N}:\alpha,\beta\le N} c_\alpha d_\beta\varphi_\alpha\otimes\psi_\beta\Big\|_{\mathcal{H}_1\otimes\mathcal{H}_2}\\
&\le \limsup_{N\to\infty}\Big\|\sum_{\beta\in\mathbb{N}:\beta\le N} d_\beta\zeta\otimes\psi_\beta-\sum_{\alpha,\beta\in\mathbb{N}:\alpha,\beta\le N} c_\alpha d_\beta\varphi_\alpha\otimes\psi_\beta\Big\|_{\mathcal{H}_1\otimes\mathcal{H}_2}\\
&\quad+\limsup_{N\to\infty}\Big\|\zeta\otimes\xi-\sum_{\beta\in\mathbb{N}:\beta\le N} d_\beta\zeta\otimes\psi_\beta\Big\|_{\mathcal{H}_1\otimes\mathcal{H}_2}\\
&\le \limsup_{N\to\infty}\Big\|\zeta-\sum_{\alpha\in\mathbb{N}:\alpha\le N} c_\alpha\varphi_\alpha\Big\|_{\mathcal{H}_1}\|\xi\|_{\mathcal{H}_2}+\|\zeta\|_{\mathcal{H}_1}\Big\|\xi-\sum_{\beta\in\mathbb{N}:\beta\le N} d_\beta\psi_\beta\Big\|_{\mathcal{H}_2}=0.
\end{aligned}$$

□

Analogously to the product of two Hilbert spaces, we can define $\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_n$, the product of n Hilbert spaces $\mathcal{H}_1,\dots,\mathcal{H}_n$ (the details are left to the reader).

Example 2.3. *A system of two particles moving in $\mathbb{R}^d$ is described by the Hilbert space $L^2(\mathbb{R}^d)\otimes L^2(\mathbb{R}^d)$. The space $L^2(\mathbb{R}^d)\otimes L^2(\mathbb{R}^d)$ is unitarily isomorphic to $L^2(\mathbb{R}^{2d})$.*

Proof. We first embed $L^2(\mathbb{R}^d)\otimes L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^{2d})$ through the linear isometric map

$$L^2(\mathbb{R}^d)\otimes L^2(\mathbb{R}^d)\ni\varphi\otimes\psi\overset{\iota}{\mapsto}\Big((x,y)\mapsto\varphi(x)\psi(y)\Big)\in L^2(\mathbb{R}^{2d}).$$

Considering the fact that ι is a linear isometry, the claim follows if we show that ι is onto. To see this, denote by $(\varphi_\alpha)_{\alpha\in\mathbb{N}}$ an orthonormal basis of $L^2(\mathbb{R}^d)$ so that $(\iota(\varphi_\alpha\otimes\varphi_\beta))_{\alpha,\beta\in\mathbb{N}}$ is an orthonormal basis of $\mathcal{S}=\iota(L^2(\mathbb{R}^d)\otimes L^2(\mathbb{R}^d))$. Now, suppose $\zeta\in L^2(\mathbb{R}^{2d})$ is s.t.

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} dxdy\,\overline{\varphi}_\alpha(x)\overline{\varphi}_\beta(y)\zeta(x,y)=0,\ \ \forall\alpha,\beta\in\mathbb{N},$$

that is $\zeta\in\mathcal{S}^\perp$. This implies that $x\mapsto\int dy\,\overline{\varphi}_\beta(y)\zeta(x,y)=0\in L^2(\mathbb{R}^d)$ (why?) so that almost surely in $x\in\mathbb{R}^d$, we have

$$\int_{\mathbb{R}^d} dy\,\overline{\varphi}_\beta(y)\zeta(x,y)=0,\ \ \forall\beta\in\mathbb{N}.$$

But this means that almost surely in $x\in\mathbb{R}^d$, we have $\zeta(x,\cdot)=0\in L^2(\mathbb{R}^d)$ so that

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} dxdy\,|\zeta(x,y)|^2=\int_{\mathbb{R}^d} dx\Big(\int_{\mathbb{R}^d} dy\,|\zeta(x,y)|^2\Big)=0.$$

We conclude that $\mathcal{S}^\perp=\{0\}$ which is equivalent to $\mathcal{S}=L^2(\mathbb{R}^{2d})$. □

Example 2.4 (Fock spaces)**.** *Let $\mathcal{H}$ be a Hilbert space. The Fock space $\mathcal{F}(\mathcal{H})$ over $\mathcal{H}$ is*

$$\mathcal{F}(\mathcal{H}) := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathcal{H}^{\otimes n} = \big\{ (\psi_n)_{n\in\mathbb{N}_0} = (\psi_0, \psi_1, \psi_2, \dots) : |\psi_0|^2 + \sum_{n=1}^{\infty} \|\psi_n\|^2_{\mathcal{H}^{\otimes n}} < \infty \big\}$$

It is a Hilbert space with the inner product $\langle \psi, \varphi \rangle_{\mathcal{F}(\mathcal{H})} = \overline{\psi}_0 \varphi_0 + \sum_{n=1}^{\infty} \langle \psi_n, \varphi_n \rangle_{\mathcal{H}^{\otimes n}}$.

In many body quantum mechanics, particles moving in $\Omega \subset \mathbb{R}^d$ (in the main part of the course we mostly consider particles moving in $\mathbb{R}^3$) fall into two classes, they are either fermions or bosons. To which symmetry class the particles belong to is related to their spin, a property we will not discuss further in these notes. To describe in particular systems of bosons properly, we need to introduce the notion of the n-fold symmetric tensor product of a Hilbert space $\mathcal{H}$. Let $\mathfrak{S}_n$ denote the permutation group of $n \in \mathbb{N}$ elements. We define S_n on the set of vectors $\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_n \in \mathcal{H}^{\otimes n}$, $\psi_i \in \mathcal{H}, i = 1, \dots, n$, by

$$S_n(\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_n) = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} \psi_{\sigma(1)} \otimes \psi_{\sigma(2)} \otimes \cdots \otimes \psi_{\sigma(n)}.$$

We extend S_n to a linear map from the set of finite linear combinations of vectors of the form $\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_n \in \mathcal{H}^{\otimes n}$ to $\mathcal{H}^{\otimes n}$ and it is not hard to see that S_n is Lipschitz continuous with Lipschitz constant L equal to $L = 1$ (in the words of section 2.3, it is a bounded, linear operator on $\mathcal{H}^{\otimes n}$). Since the set of finite linear combinations of product wave functions is by definition dense in $\mathcal{H}^{\otimes n}$, S_n extends uniquely to a continuous map from $\mathcal{H}^{\otimes n}$ to itself. We define $\mathcal{H}^{\otimes_s n} = S_n(\mathcal{H}^{\otimes n})$ which is called the *n-fold symmetric tensor product of $\mathcal{H}$.* $\mathcal{H}_s^{\otimes n}$ is a Hilbert subspace of $\mathcal{H}^{\otimes n}$.

Example 2.5. *A system of $N \in \mathbb{N}$ (identical, spinless) bosons moving in $\mathbb{R}^d$ is described by a wave function $\psi \in L^2_s(\mathbb{R}^{dN}) = S_N\big(L^2(\mathbb{R}^{dN})\big)$. It is characterized by the property that for every $\sigma \in \mathfrak{S}_N$ and for a.e. $(x_1, x_2, \dots, x_N) \in \mathbb{R}^{dN}$, it holds true that*

$$\psi(x_1, x_2, \dots, x_N) = \psi\big(x_{\sigma(1)}, x_{\sigma(2)}, \dots, x_{\sigma(N)}\big)$$

Example 2.6 (Bosonic Fock spaces)**.** *Let $\mathcal{H}$ be a Hilbert space. The bosonic Fock space $\mathcal{F}_s(\mathcal{H})$ over $\mathcal{H}$ is the Hilbert space defined by $\mathcal{F}_s(\mathcal{H}) = \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathcal{H}^{\otimes_s n} \subset \mathcal{F}(\mathcal{H})$.*

2.2 Closed, Symmetric and Self-Adjoint Operators

In quantum mechanics, physically measurable quantities, called observables, are described by self-adjoint operators. Loosely speaking, the idea is as follows: consider a finite dimensional, complex Hilbert space $\mathcal{H} \simeq \mathbb{C}^n$ and a Hermitean matrix $A : \mathbb{C}^n \to \mathbb{C}^n$. From linear algebra, we know that A is unitarily equivalent to a diagonal matrix and that its n eigenvalues are real-valued. Denote by $\varphi_1, \dots, \varphi_n$ an orthonormal eigenbasis of A corresponding to the eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. If A is an observable, then the eigenvalues of A are interpreted as the possible values of that observable and the postulates of quantum mechanics assign to each value a certain probability for finding it: indeed, if the state of the quantum system is described by $\psi \in \mathbb{C}^n$, $\|\psi\|_{\mathbb{C}^n} = 1$, the spectral measure μ_ψ^A associated to A and $\psi \in \mathbb{C}^n$ is defined on $\mathcal{P}(\sigma(A))$ with $\sigma(A) = \{\lambda_i, i = 1, \dots, n\}$ by

$$\mu_\psi^A(\Omega) = \sum_{i:\lambda_i \in \Omega \subset \sigma(A)} |\langle \psi, \varphi_i \rangle_{\mathbb{C}^n}|^2$$

The expected value of A is given by $\langle \psi, A\psi \rangle$. Note that this is equal to $\mathbb{E}(\xi_A)$ where ξ_A is the random variable $\lambda_i \mapsto \xi_A(\lambda_i) = \lambda_i$ on the probability space $(\sigma(A), \mathcal{P}(\sigma(A)), \mu_\psi^A)$.

In typical cases, the Hilbert space $\mathcal{H}$ describing the system is not finite dimensional. Also, observables typically do not correspond to bounded linear operators (like matrices on finite dimensional Hilbert spaces), but are in general unbounded (for instance, we need differential operators to describe momentum and kinetic energy of a quantum particle). In such a setting, the right class of operators to describe physically measurable quantities consists of self-adjoint operators. In analogy to the above, for such operators it is possible to construct appropriate Borel probability measures giving the probability for finding the value of an observable in a measurable subset of $\mathbb{R}$ (see section 2.4).

A linear operator $A : D(A) \to \mathcal{H}$ is a linear map from a linear subspace $D(A) \subset \mathcal{H}$, called the domain of A, to $\mathcal{H}$. A is densely defined if $D(A)$ is dense in $\mathcal{H}$. We always consider densely defined operators unless stated explicitly otherwise. A linear operator $A : D(A) \to \mathcal{H}$ is bounded if its operator norm is finite, that is

$$\|A\|_{\mathcal{L}(\mathcal{H})} = \|A\| = \sup_{\psi \in D(A), \|\psi\|_{\mathcal{H}} = 1} \|A\psi\|_{\mathcal{H}} < \infty$$

If A is bounded, it is in particular Lipschitz continuous and can be extended uniquely to a bounded operator on $\mathcal{H}$. A linear operator is called unbounded if it is not bounded.

Example 2.7. *Consider $L^2(\mathbb{R})$ and let $\widehat{x} : C_c^\infty(\mathbb{R}) \to L^2(\mathbb{R})$ denote the position operator, defined by $(\widehat{x}(\varphi))(x) = x\varphi(x)$, $x \in \mathbb{R}$. Then $\hat{x}$ is densely defined and unbounded.*

Proof. It is a standard fact that $C_c^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R})$. The fact that $\hat{x}$ is unbounded can be proved, for instance, by considering some $0 \leq \varphi \in C_c^\infty((-1, 1))$ with $\|\varphi\|_2 = 1$ and its translates $\varphi_n = \varphi(\cdot - n) \in C_c^\infty((n - 1, n + 1)$. Then $\|\varphi_n\|_2 = 1$ for all $n \in \mathbb{N}$ and

$$\|\widehat{x}\varphi_n\|_2^2 = \int_{(n-1,n+1)} dx\, x^2 |\varphi_n(x)|^2 \geq Cn^2 \to \infty \quad \text{as} \quad n \to \infty.$$

□

Problem 2.2. *Show that $i\nabla : C_c^\infty(\mathbb{R}^d) \to \left(L^2(\mathbb{R}^d)\right)^d$ and $-\Delta = -\sum_{i=1}^d \partial_i^2 : C_c^\infty(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ are unbounded.*

Let $A : D(A) \to \mathcal{H}$ be a linear operator. The resolvent set $\rho(A)$ of A is defined by

$$\rho(A) = \{z \in \mathbb{C} : (A - z) \text{ has a bounded inverse } (A - z)^{-1} : \mathcal{H} \to D(A)\} \tag{2.1}$$

If $z \in \rho(A)$, we call $R_z(A) = (A - z)^{-1}$ the resolvent of A at $z \in \mathbb{C}$. The spectrum $\sigma(A)$ of A is defined by

$$\sigma(A) = \mathbb{C} \setminus \rho(A) \tag{2.2}$$

The discrete spectrum $\sigma_{\mathrm{d}}(A) \subset \sigma(A)$ of A is the set of isolated eigenvalues of A of finite multiplicity. The essential spectrum $\sigma_{\mathrm{ess}}(A)$ is defined by $\sigma_{\mathrm{ess}}(A) = \sigma(A) \setminus \sigma_{\mathrm{d}}(A)$.

Theorem 2.1. *Let $A : D(A) \to \mathcal{H}$ be a linear operator. Then $\rho(A) \subset \mathbb{C}$ is open, $\sigma(A) \subset \mathbb{C}$ is closed and the function $z \mapsto R_z(A)$ is analytic in $\rho(A)$. Moreover, the set $\{R_z(A) : z \in \rho(A)\}$ is a set of commuting operators and it holds true that*

$$R_\lambda(A) - R_\mu(A) = (\lambda - \mu) R_\lambda(A) R_\mu(A) \qquad (\forall\, \mu, \lambda \in \rho(A))$$

Remark. *Analyticity of $z \mapsto R_z(A)$ in Theorem 2.1 means that for any $z_0 \in \rho(A)$, the operator-valued map $z \mapsto R_z(A)$ has a norm-convergent power series expansion in $z - z_0$ for all $z \in \rho(A)$ in some neighborhood around z_0.*

Proof. That $[R_\mu(A), R_\lambda(A)] = 0$ follows from $[(A - \mu), (A - \lambda)] = 0$, which implies that $R_\mu(A)R_\lambda(A)$ is the inverse to $(A - \mu)(A - \lambda)$, i.e. equal to $R_\lambda(A)R_\mu(A)$. The remaining claims follow from a geometric series argument and the useful identity

$$A - z = (A - z_0)\big(1 - (A - z_0)^{-1}(z - z_0)\big)$$

for suitable $z, z_0 \in \rho(A)$. Indeed, if $z_0 \in \rho(A)$, then the previous identity shows that $B_r(z_0) \subset \rho(A)$ for $r = \|R_{z_0}(A)\|$, because for $z \in B_r(z_0)$, we have

$$\big(1 - (A - z_0)^{-1}(z - z_0)\big)^{-1} = \sum_{k \geq 0} R_{z_0}^k (z - z_0)^k$$

Note that the r.h.s. in the previous equation is a norm-convergent series in $z - z_0$. This proves that $\rho(A)$ is open, $\sigma(A)$ is closed and that $z \mapsto R_z(A)$ is analytic in $\rho(A)$. The resolvent identity follows from

$$R_\lambda(A) - R_\mu(A) = R_\lambda(A)\big(A - \mu - A + \lambda\big)R_\mu(A) = (\lambda - \mu) R_\lambda(A) R_\mu(A).$$

□

As mentioned earlier, we will need to work with unbounded operators like differential operators. Typically, we start with a domain like $C_c^\infty(\mathbb{R}^d)$ on which we understand the action of the operator very well - in order to be able to talk about self-adjoint realizations of a given operator, though, we need in general to extend the operator onto larger domains (and possibly add some boundary condition, see below for examples and more details). For such extensions, we typically want to satisfy at least some minimal requirement: we call an (not necessarily densely defined) operator A closed if its graph

$$\Gamma(A) = \big\{(\psi, A\psi) : \psi \in D(A)\big\}$$

is closed as a subset of $\mathcal{H} \times \mathcal{H}$. In other words, A is closed if and only if

$$\psi_n \to \psi \in \mathcal{H} \quad \text{and} \quad A\psi_n \to \phi \in \mathcal{H} \quad \text{as} \quad n \to \infty$$

implies that

$$\psi \in D(A) \quad \text{and} \quad A\psi = \phi.$$

Equivalently, $D(A)$ equipped with $\|\cdot\|_{D(A)} = \|\cdot\|_{\mathcal{H}} + \|A(\cdot)\|_{\mathcal{H}}$ is a Banach space.

Problem 2.3. *Find an explicit example of an operator which is not closed.*

We call A_2 an *extension* of A_1 if $\Gamma(A_1) \subset \Gamma(A_2)$, which means that $D(A_1) \subset D(A_2)$ and $(A_2)_{|D(A_1)} = A_1$. We say that an operator is *closable* if it has a closed extension.

Lemma 2.2. *If A is closable, it has a smallest, closed extension $\overline{A}$ with $\Gamma(\overline{A}) = \overline{\Gamma(A)}$. Moreover, A is closable if and only if $\psi_n \to 0$ and $A\psi_n \to \phi$ as $n \to \infty$ implies $\phi = 0$.*

Proof. Let A be closable, then it has a closed extension B, by definition. This means $\Gamma(A) \subset \Gamma(B)$ and $\Gamma(B)$ is a closed, linear subspace in $\mathcal{H} \times \mathcal{H}$. Now, consider the closure $\overline{\Gamma(A)} \subset \Gamma(B)$. Since $\Gamma(B)$ is the graph of a linear operator, it has the property that

$$(0, \phi) \in \Gamma(B) \quad \text{implies} \quad \phi = 0.$$

As a subset of $\Gamma(B)$, also $\overline{\Gamma(A)}$ has this property and it is also clear that $\Gamma(A)$ (and thus $\overline{\Gamma(A)}$) is a linear subspace of $\mathcal{H} \times \mathcal{H}$. Define $\overline{A} : D(\overline{A}) \to \mathcal{H}$ by

$$D(\overline{A}) = \pi_1(\overline{\Gamma(A)}), \quad \overline{A}\psi = \pi_2\big(\{\psi\} \times \mathcal{H} \cap \overline{\Gamma(A)}\big) \ \forall \psi \in D(\overline{A}).$$

Due to the linearity of $\overline{\Gamma(A)}$, the domain $D(\overline{A})$ is a linear space and due to the property above, $\overline{A}$ is well-defined: if $(\psi, \phi), (\psi, \phi') \in \overline{\Gamma(A)}$, then $(0, \phi - \phi') \in \overline{\Gamma(A)}$ and thus $\phi = \phi'$. In other words, for every $\psi \in D(\overline{A})$, there is a unique $\phi (= \overline{A}\psi) \in \mathcal{H}$ such that $(\psi, \phi) \in \overline{\Gamma(A)}$. The linearity of $\overline{A}$ follows from this with the linearity of $\overline{\Gamma(A)}$.

In conclusion, $\overline{A}$ is a closed linear operator with $\Gamma(\overline{A}) = \overline{\Gamma(A)}$, in particular it is a closed extension of A. Any other closed extension B has the property that $\Gamma(\overline{A}) \subset \Gamma(B)$, so $\overline{A}$ is the smallest closed linear extension of A.

For the second statement, notice that A is closable if and only if $\overline{\Gamma(A)}$ has the property that $(0, \phi) \in \overline{\Gamma(A)}$, then $\phi = 0$. Both the if- and the only-if-statements follow from the previous arguments. ☐

Example 2.8. *([55, Problem 1]). Let $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$ be an orthonormal basis of a separable, infinite dimensional Hilbert space $\mathcal{H}$. Let $\varphi_\infty \in \mathcal{H}$ be an element that is not a finite linear combination of the basis elements $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$. On the dense subspace $D(A) = \operatorname{span}(\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\} \cup \{\varphi_\infty\})$, we can define the linear operator $A : D(A) \to \mathcal{H}$ by*

$$A(\lambda\varphi_\infty + \sum_{n=1}^{N} \mu_n \varphi_n) = \lambda\varphi_\infty$$

Then $\overline{\Gamma(A)}$ is not the graph of a linear operator, because $(\varphi_\infty, \varphi_\infty), (\varphi_\infty, 0) \in \overline{\Gamma(A)}$.

Example 2.9. *(Linear differential operators are closable). Consider a linear differential operator* $A = \sum_{|\alpha|\leq N} \lambda_\alpha \partial^\alpha$ *on* $C_c^\infty(\mathbb{R}^d)$*, where* $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$ *and*

$$\partial^\alpha = \partial_1^{\alpha_1} \ldots \partial_d^{\alpha_d}.$$

Then $A : C_c^\infty(\mathbb{R}^d) \subset L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ *is closable.*

Proof. We show that $\psi_n \to 0$ and $A\psi_n \to \phi \in L^2(\mathbb{R}^d)$ as $n \to \infty$ implies $\phi = 0$. Let $\zeta \in C_c^\infty(\mathbb{R}^d)$, then by integration by parts

$$\begin{aligned}\langle \zeta, \phi \rangle_2 = \lim_{n\to\infty} \langle \zeta, A\psi_n \rangle &= \lim_{n\to\infty} \int_{\mathbb{R}^d} dx\, \overline{\Big(\sum_{|\alpha|\leq N} (-1)^{\sum_{i=1}^d \alpha_i} \lambda_\alpha \partial^\alpha \zeta \Big)} \psi_n(x) \\ &= \lim_{n\to\infty} \Big\langle \Big(\sum_{|\alpha|\leq N} (-1)^{\sum_{i=1}^d \alpha_i} \overline{\lambda}_\alpha \partial^\alpha \zeta \Big), \psi_n \rangle_2 = 0.\end{aligned}$$

Hence, $\phi = 0$ by density of $C_c^\infty(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$, so that A is closable. □

Next, we introduce the adjoint of a linear operator. Let $A : D(A) \to \mathcal{H}$ be a densely defined operator on $\mathcal{H}$ and define $D(A^*)$ by

$$D(A^*) = \big\{ \varphi \in \mathcal{H} : \exists\, \eta \in \mathcal{H} \text{ with } \langle \varphi, A\psi \rangle_{\mathcal{H}} = \langle \eta, \psi \rangle_{\mathcal{H}} \;\; \forall \psi \in D(A) \big\} \subset \mathcal{H}$$

Given $\varphi \in D(A^*)$ s.t. $\langle \varphi, A\psi \rangle_{\mathcal{H}} = \langle \eta, \psi \rangle_{\mathcal{H}}$ for all $\psi \in D(A)$ we set $A^*\varphi = \eta$. The operator $A^* : D(A^*) \to \mathcal{H}$ is a well-defined (why?), linear operator and called the *adjoint* of A. If A^* is densely defined, we let $A^{**} = (A^*)^*$. For the notion of self-adjointness, we need to know whether A^* is densely defined. In general, this need not to be the case.

Example 2.10. *Suppose f is a bounded, measurable function, but such that* $f \notin L^2(\mathbb{R})$. *Define* $D(A) = \{\psi \in L^2(\mathbb{R}) : \int_{\mathbb{R}} dx\, \overline{f}(x)\psi(x) \in \mathbb{C}\}$. *Then $D(A)$ is dense in* $L^2(\mathbb{R})$ *(why?) and on $D(A)$ we set* $A\psi = (\int_{\mathbb{R}} dx\, \overline{f}(x)\psi(x))\psi_0$*, for some fixed* $0 \neq \psi_0 \in L^2(\mathbb{R})$. *Let's consider the adjoint A^* of A. If* $\varphi \in D(A^*)$*, then*

$$\langle A^*\varphi, \psi \rangle_2 = \langle \varphi, A\psi \rangle_2 = \Big(\int_{\mathbb{R}} dx\, f(x)\psi(x) \Big) \langle \varphi, \psi_0 \rangle_2 = \int_{\mathbb{R}} dx\, \big(\langle \varphi, \psi_0 \rangle_2 \big) \overline{f}(x)\psi(x)$$

for all $\psi \in D(A)$. *This means that* $A^*\varphi = \overline{\langle \varphi, \psi_0 \rangle_2} f$, *but* $f \notin L^2(\mathbb{R})$, *so that we must have* $\langle \varphi, \psi_0 \rangle_2 = 0$. *In particular, $D(A^*)$ is not dense, but consists of* $\{\psi_0\}^\perp$.

Theorem 2.2. *Let* $A : D(A) \to \mathcal{H}$ *be a densely defined operator on a Hilbert space* $\mathcal{H}$. *Then the following holds true.*

i) $A^* : D(A^*) \to \mathcal{H}$ *is a closed operator.*

ii) A is closable if and only if $D(A^*)$ is dense, and in this case $\overline{A} = A^{**}$.

iii) If A is closable, then $(\overline{A})^* = A^*$.

Proof. i) Consider $\mathcal{H} \times \mathcal{H}$ as Hilbert space with the inner product

$$\langle(\psi_1, \psi_2), (\varphi_1, \varphi_2)\rangle_{\mathcal{H}\times\mathcal{H}} = \langle\psi_1, \varphi_1\rangle_{\mathcal{H}} + \langle\psi_2, \varphi_2\rangle_{\mathcal{H}} \quad (\forall \psi_1, \psi_1, \varphi_1, \varphi_2 \in \mathcal{H})$$

Define $V : \mathcal{H} \times \mathcal{H} \to \mathcal{H} \times \mathcal{H}$ by

$$V(\psi, \varphi) = (-\varphi, \psi).$$

Then V is clearly unitary. As a consequence, $V(E)^\perp = V(E^\perp)$ for every subspace $E \subset \mathcal{H}\times\mathcal{H}$. Indeed, if $\langle\xi, V\eta\rangle_{\mathcal{H}\times\mathcal{H}} = \langle V^*\xi, \eta\rangle_{\mathcal{H}\times\mathcal{H}} = 0$ for all $\eta \in E$, then $\xi = V(V^*\xi) \in V(E^\perp)$. On the other hand, if $\xi = V(\widetilde{\xi}) \in V(E^\perp)$, then $\langle\xi, V\eta\rangle_{\mathcal{H}\times\mathcal{H}} = \langle V\widetilde{\xi}, V\eta\rangle_{\mathcal{H}\times\mathcal{H}} = \langle\widetilde{\xi}, \eta\rangle_{\mathcal{H}\times\mathcal{H}} = 0$ for all $\eta \in E$, i.e. $\xi \in V(E)^\perp$.

Now, denote by $\Gamma(A)$ the graph of A. We claim that $V(\Gamma(A))^\perp = \Gamma(A^*)$, showing that $\Gamma(A^*)$ is closed. Indeed, $(\xi, \varphi) \in V(\Gamma(A))^\perp$ if and only if

$$0 = \langle(\xi, \varphi), (-A\psi, \psi)\rangle_{\mathcal{H}\times\mathcal{H}} = -\langle\xi, A\psi\rangle_{\mathcal{H}} + \langle\varphi, \psi\rangle_{\mathcal{H}}, \quad \forall\psi \in D(A),$$

which is the case if and only if $\langle\xi, A\psi\rangle_{\mathcal{H}} = \langle\varphi, \psi\rangle_{\mathcal{H}}$ for all $\psi \in D(A)$. The latter statement holds true if and only if $\xi \in D(A^*)$ and $\varphi = A^*\xi$, i.e. $(\xi, \varphi) \in \Gamma(A^*)$.

ii) Assume that A^* is densely defined. Since A is linear, $\Gamma(A)$ is a linear subspace of $\mathcal{H} \times \mathcal{H}$. With $V^2 = -\mathbf{1}_{\mathcal{H}}$ and the proof of i), this implies

$$\overline{\Gamma(A)} = (\Gamma(A)^\perp)^\perp = ((V^2(\Gamma(A)))^\perp)^\perp = (V((V(\Gamma(A))^\perp)))^\perp = (V(\Gamma(A^*))^\perp = \Gamma(A^{**})$$

This shows that $\overline{\Gamma(A)}$ is the graph of A^{**}, so that A is closable with $\overline{A} = A^{**}$.

If we assume on the other hand that $D(A^*)$ is not dense, we may consider an element $0 \neq \psi \in D(A^*)^\perp$. It then follows that $(\psi, 0) \in \Gamma(A^*)^\perp$ which implies that $V(\Gamma(A^*)^\perp) = (V(\Gamma(A^*)))^\perp$ can not be the graph of a linear operator, because $(0, \psi) \in V(\Gamma(A^*)^\perp)$. But by the previous step, $(V(\Gamma(A^*)))^\perp = \overline{\Gamma(A)}$, so that A is not closable.

iii) If A is closable, $D(A^*)$ is dense in $\mathcal{H}$ and A^* is closed s.t.

$$A^* = \overline{(A^*)} \overset{ii)}{=} (A^*)^{**} = ((A^*)^*)^* = (A^{**})^* \overset{ii)}{=} (\overline{A})^*$$

□

In contrast to the finite-dimensional case, in infinite dimensions there is an important distinction between symmetric and self-adjoint operators. The spectral theorem mentioned earlier applies to self-adjoint operators, but not to symmetric operators which are not self-adjoint. Having a self-adjoint realization of a given unbounded operator is often intimately connected with choosing an appropriate domain. In fact, spectral properties of unbounded operators are sensitive w.r.t. the choice of the domain.

Consider for example the operator $A = i\partial_x$ which represents the momentum of a quantum particle[1]. Since observables correspond to self-adjoint operators, it is important to understand the self-adjoint realizations of A. We approach this question step by step, illustrating some basic difficulties when trying to define A as a self-adjoint operator.

[1]More precisely, the momentum operator $\hat{p}$ in quantum mechanics corresponds to the generator of the unitary group of translations. It corresponds to the physical quantity that is preserved in closed

Example 2.11. *Consider $A : H^1([0,1]) \to L^2([0,1])$ defined by $A\psi = i\partial_x\psi$. Then the spectrum of A is given by the whole plane $\sigma(A) = \mathbb{C}$. Indeed, every $z \in \mathbb{C}$ is an eigenvalue of A with a possible eigenfunction given by $x \mapsto e^{-izx} \in H^1([0,1])$. Notice also that A is closed, because $H^1([0,1])$ with the graph norm is a Banach space.*

At this point, let us recall that any $\psi \in H^1((0,1))$ admits an absolutely continuous representative $\widetilde{\psi} \in C([0,1])$, which satisfies

$$\widetilde{\psi}(b) = \widetilde{\psi}(a) + \int_a^b ds\, \psi'(s)$$

for every $a, b \in [0,1]$. In particular, this gives meaning to $\psi(0)$ and $\psi(1)$. In the following we therefore identify implicitly $H^1([0,1])$ with $H^1((0,1))$, including the boundary of $(0,1)$ as a reminder of this fact.

Example 2.12. *Consider $A : D(A) \to L^2([0,1])$ defined by $A\psi = i\partial_x\psi$, as in the previous example, but on the modified domain*

$$D(A) = \{\psi \in H^1([0,1]) : \psi(0) = 0\}.$$

The operator $A : D(A) \to L^2([0,1])$ has empty spectrum.

Proof. We will show that $A - z$ is invertible for every $z \in \mathbb{C}$, with bounded inverse. Indeed, given $\varphi \in L^2([0,1])$, this amounts to solving the ODE

$$\partial_x\psi = -iz\psi - i\varphi \quad \text{with} \quad \psi(0) = 0.$$

Motivated by Duhamel's formula, we analyze the operator $S_z : L^2([0,1]) \to D(A)$

$$(S_z\varphi)(x) = -i\int_0^x ds\, e^{-iz(x-s)}\varphi(s).$$

Then S_z is a bounded operator, because

$$\begin{aligned}\|S_z\varphi\|_2^2 \le \|S_z\varphi\|_\infty^2 &\le \left(\sup_{x\in[0,1]}\int_0^1 ds\, |e^{-iz(x-s)}\varphi(s)|\right)^2 \\ &\le \left(\sup_{x\in[0,1]}\int_0^1 ds\, |e^{-iz(x-s)}|^2\right)\|\varphi\|_2^2 \le C_z\|\varphi\|_2^2,\end{aligned}$$

by Cauchy-Schwarz, where $C_z > 0$ is some finite constant. Moreover, we have

$$(A - z)S_z\varphi = \left(\varphi - (-i^2 z)\, i\int_0^{\cdot} ds\, e^{-iz(\cdot - s)}\varphi(s)\right) - zS_z\varphi = \varphi,$$

---

systems due to the homogeneity of Euclidean space. For suitable φ, we therefore have

$$(\hat{p}\varphi)(x) = -i\lim_{y\to 0}\frac{1}{y}(U(y)\varphi - \varphi)(x) = -i\lim_{y\to 0}\frac{1}{y}(\varphi(x-y) - \varphi(x)) = (i\partial_x\varphi)(x),$$

interpreting $U(y) = e^{-i\hat{p}y}$ (see the section on the spectral theorem below for the rigorous definition of the strongly-continuous unitary group $(U(y))_{y\in\mathbb{R}}$).

that is $(A-z)S_z = \mathbf{1}_{L^2([0,1])}$, as well as

$$\big(S_z(A-z)\varphi\big)(x) = \int_0^x ds\, e^{-iz(x-s)}(\partial_x\varphi - iz\varphi)(s)$$
$$= \varphi(x) - e^{-izx}\varphi(0) + \int_0^x ds\, e^{-iz(x-s)}(iz\varphi - iz\varphi)(s) = \varphi(x)$$

for all $\varphi \in D(A)$, by integration by parts. Thus, $S_z(A-z) = \mathbf{1}_{|D(A)}$. This means that $S_z = R_z = (A-z)^{-1} : L^2([0,1]) \to D(A)$ is the resolvent of A at $z \in \mathbb{C}$. □

The previous two examples show that more care needs to be taken in order to define $A\psi = i\partial_x\psi$ as a self-adjoint operator. It turns out that the previous examples do not even provide symmetric versions of A. We say that a linear operator $A : D(A) \to \mathcal{H}$ is symmetric if $A \subset A^*$ which means that $D(A) \subset D(A^*)$ and $A^*_{|D(A)} = A$. This is equivalent to the requirement that

$$\langle \psi, A\varphi \rangle_{\mathcal{H}} = \langle A\psi, \varphi \rangle_{\mathcal{H}}$$

for all $\psi, \varphi \in D(A)$. An operator is called self-adjoint if $A = A^*$ (i.e. if $A \subset A^*$ and $A^* \subset A$), that is, if A is symmetric and $D(A) = D(A^*)$. If $A : D(A) \to \mathcal{H}$ is symmtric, it is closable by Theorem 2.2 ii), because $D(A^*) \supset D(A)$ is dense in $\mathcal{H}$. In this case, the closure of A is given by $\overline{A} = A^{**}$. Since A^* is also a closed extension of A, we deduce

$$A \subset A^{**} \subset A^*$$

for any symmetric operator $A : D(A) \to \mathcal{H}$. If A is also closed, we have

$$A = A^{**} \subset A^*$$

and if A is self-adjoint, we have that $A = A^{**} = A^*$.

We call a symmetric operator $A : D(A) \to \mathcal{H}$ essentially self-adjoint if its closure $\overline{A} : D(\overline{A}) \to \mathcal{H}$ is self-adjoint and if $A : D(A) \to \mathcal{H}$ is closed, we call $D \subset D(A)$ a core for A if $\overline{A_{|D}} = A$. If A is essentially self-adjoint, it has a unique self-adjoint extension: indeed, if B is some self-adjoint extension, we have $A^{**} \subset B$ and $B = B^* \subset (A^{**})^* = A^{**} \subset B$. An operator $A : D(A) \to \mathcal{H}$ is essentially self-adjoint if and only if $A \subset A^{**} = A^*$.

Problem 2.4. *Check, more generally, that if $A \subset B$ are both densely defined linear operators and B extends A, then A^* extends B^*, $B^* \subset A^*$.*

Example 2.13. *Let's consider again $A = i\partial_x$ and let's define it on $D(A)$, where*

$$D(A) = \{\psi \in H^1([0,1]) : \psi(0) = 0 = \psi(1)\}.$$

We might suspect that, the more boundary conditions we impose on A, the fewer restrictions we have on the domain of A^*. In fact, we have $A \subset A^*$ with $D(A^*) = H^1([0,1])$.

Proof. To see that A is symmetric, let $\varphi, \psi \in D(A)$, then integration by parts implies

$$\langle \varphi, A\psi \rangle_2 = \int_0^1 dx\, \overline{\varphi}(x)(i\partial_x \psi)(x) = i\, \overline{\varphi}\, \psi \Big|_0^1 - i \int_0^1 dx\, (\partial_x \overline{\varphi})(x)\psi(x) = \langle A\varphi, \psi \rangle_2.$$

Hence, $A \subset A^*$. To compute $D(A^*)$, we notice that the same computation involving integration by parts shows that $H^1([0,1]) \subset D(A^*)$. On the other hand, suppose that $\psi \in D(A^*)$. By definition, this means that there exists $\eta\,(= A^*\psi) \in L^2([0,1])$ such that

$$\langle \psi, A\varphi \rangle_2 = i \int_0^1 \overline{\psi}(x)(\partial_x \varphi)(x) = \int_0^1 \overline{\eta}(x)\varphi(x)$$

for all $\varphi \in D(A)$. In particular, the last identity holds true for all $\varphi \in C_c^\infty((0,1))$ and this just means that the distributional derivative of ψ can be identified with $-i\eta \in L^2([0,1])$, i.e. $D(A^*) \subset H^1([0,1])$. By the Sobolev embedding in $\mathbb{R}$, we know additionally that ψ has the absolutely continuous representative

$$[0,1] \ni x \mapsto \psi(x) = \psi(0) - i \int_0^x ds\, \eta(s) \in H^1([0,1]).$$

□

Example 2.14. *This time we define $A = i\partial_x$ on the domain*

$$D(A) = \{\psi \in H^1([0,1]) : \psi(0) = \psi(1)\},$$

then $A : D(A) \to L^2([0,1])$ is self-adjoint, i.e. $A = A^*$.

Proof. Integration by parts shows as before that $A \subset A^*$. To show the other direction, we argue as in the previous example to see that $D(A^*) \subset H^1([0,1])$ with $A^*\psi = i\partial_x\psi$ for all $\psi \in D(A^*)$, using that $C_c^\infty((0,1)) \subset D(A)$. But then, if $\psi \in D(A^*)$, we can choose $\varphi = 1 \in D(A)$ and conclude

$$0 = \langle \psi, A\varphi \rangle_2 = i \int_0^1 ds\, (\partial_x \overline{\psi})(s) = i(\overline{\psi}(1) - \overline{\psi}(0)),$$

so that $\psi \in D(A)$. □

Problem 2.5. *There are in fact uncountably many different self-adjoint extensions of $A = i\partial_x$. Prove that $A : D(A) \to L^2([0,1])$ is self-adjoint if we consider it on*

$$D(A) = \{\psi \in H^1([0,1]) : \psi(0) = \alpha\, \psi(1)\},$$

where $\alpha \in \mathbb{C}$ is fixed and such that $|\alpha| = 1$.

As a final remark with regards to the previous examples, we mention that the closed symmetric extensions of a given closed symmetric operator, and the question whether or not it admits self-adjoint extensions, can be characterized precisely by using the notion of *deficiency indices*. We refer the interested reader to [56, Chapter X.1].

Theorem 2.3. *Let $A : D(A) \to \mathcal{H}$ be a closed, symmetric operator on a Hilbert space $\mathcal{H}$. Then the following holds true.*

i) We have that $\mathrm{ran}(z-A)^{\perp} = \ker(\bar{z}-A^*)$ *and* $\dim(\ker(z-A^*))$ *is constant throughout the open upper and lower half-planes in* $\mathbb{C}$.

ii) The spectrum of A is equal to one of the following subsets of $\mathbb{C}$: the closed upper half-plane, the closed lower half-plane, the entire plane or a subset of the real line.

iii) A is self-adjoint if and only if $\sigma(A) \subset \mathbb{R}$.

Proof. Before we start with the proof of *i)*, let $z = \nu + i\mu \in \mathbb{C}$ s.t. $\mu \neq 0$. For $\varphi \in D(A)$, we have by the symmetry of A and Cauchy-Schwarz

$$\|(z-A)\varphi\|_{\mathcal{H}}^2 = \nu^2\|\varphi\|_{\mathcal{H}}^2 + \|A\varphi\|_{\mathcal{H}}^2 - 2\nu\langle\varphi, A\varphi\rangle_{\mathcal{H}} + \mu^2\|\varphi\|_{\mathcal{H}}^2 \geq \mu^2\|\varphi\|_{\mathcal{H}}^2 \tag{2.3}$$

We deduce from here and the closedness of A that $\mathrm{ran}(z-A) \subset \mathcal{H}$ is closed, that $(A-z)$ is injective whenever $\mathrm{Im}(z) \neq 0$ and that $\|R_z(A)\|_{op} \leq |\mathrm{Im}(z)|^{-1}$ if $z \in \rho(A)$.

i) The equality

$$\ker(z - A^*) = \mathrm{ran}(\overline{z} - A)^{\perp} \tag{2.4}$$

follows from $\langle\psi, (\overline{z}-A)\varphi\rangle_{\mathcal{H}} = 0$ for all $\varphi \in D(A)$ if and only if $(z-A^*)\psi = (\overline{z}-A)^*\psi = 0$.

Given $z = \nu + i\mu \in \mathbb{C}\setminus\mathbb{R}$ as above, we show that $\dim(\ker(z-A^*))$ is locally constant. To this end, consider $w \in \mathbb{C}$ and let $\psi \in \ker((z+w)-A^*)$, $\|\psi\|_{\mathcal{H}} = 1$. Now suppose that $\psi \in \ker(z-A^*)^{\perp}$, that is, $\langle\psi,\varphi\rangle_{\mathcal{H}} = 0$ for all $\varphi \in \ker(z-A^*)$. By (2.4) and the closedness of $\mathrm{ran}(\overline{z}-A)$, this implies that $\psi \in (\mathrm{ran}(\overline{z}-A)^{\perp})^{\perp} = \mathrm{ran}(\overline{z}-A)$. Hence, there exists some $\xi \in D(A)$ with $(\overline{z}-A)\xi = \psi$ so that, by (2.3),

$$0 = \langle(z+w-A^*)\psi, \xi\rangle_{\mathcal{H}} = \|\psi\|_{\mathcal{H}}^2 + \overline{w}\langle\psi,\xi\rangle_{\mathcal{H}} \geq 1 - |w|\|\xi\|_{\mathcal{H}} \geq 1 - |\mu|^{-1}|w|$$

Obviously, the last inequality gives a contradiction if $|w| < |\mu|$ in which case therefore

$$\ker((z+w)-A^*) \cap \ker(z-A^*)^{\perp} = \{0\}$$

But this implies

$$m = \dim(\ker((z+w)-A^*)) \leq \dim(\ker(z-A^*)) = n.$$

Indeed, assume w.l.o.g. that m is finite. Denoting by $P : \ker((z+w)-A^*) \to \ker(z-A^*)$ the orthogonal projection onto $\ker(z-A^*)$, restricted to $\ker((z+w)-A^*)$, the rank theorem implies $m = \dim\ker(P) + \dim\mathrm{ran}(P)$. By the above equation, however, $\dim\ker(P) = \{0\}$, because $\ker(P) = \ker((z+w)-A^*) \cap \ker(z-A^*)^{\perp} = \{0\}$. But then $\mathrm{ran}(P) \subset \ker(z-A^*)$ contains m linearly independent vectors so that $m \leq n$.

Now, if we switch the roles of z and $z+w$ and assume $|w| < \frac{|\mu|}{2}$, we also conclude that $\dim(\ker((z+w)-A^*)) \geq \dim(\ker(z-A^*))$. Indeed, switching the roles of z and $z+w$ implies as above

$$0 = \langle(z-A^*)\psi,\xi\rangle_{\mathcal{H}} \geq \ 1 - |\mu + \mathrm{Im}\, w|^{-1}|w| \geq 1 - 2|\mu|^{-1}|w|$$

which is a contradiction if $|w| < \frac{|\mu|}{2}$. Thus $\dim(\ker((z+w)-A^*)) \geq \dim(\ker(z-A^*))$ and hence $\dim(\ker((z+w)-A^*)) = \dim(\ker(z-A^*))$ for $|w| \leq \frac{|\mu|}{2}$.

ii) The bound (2.3) implies that $(z-A)$ is injective for any $z \in \mathbb{C}\setminus\mathbb{R}$ and the inverse $(z-A)^{-1} : \operatorname{ran}(z-A) \to D(A)$ is defined on all of $\mathcal{H}$ if and only if

$$\dim(\ker(\overline{z}-A^*)) = 0 = \dim \operatorname{ran}(z-A)^{\perp}.$$

In the latter case, $z \in \rho(A)$ with $\|R_z(A)\|_{op} \leq |\operatorname{Im} z|^{-1}$, by (2.3). By part *i*), we know that $\dim(\ker(\overline{z}-A^*))$ is locally constant around $z \in \mathbb{C}$ with $\operatorname{Im} z \neq 0$. This implies that the upper and lower half planes are both either entirely contained in $\rho(A)$ (if e.g. $\dim(\ker(i-A^*)) = 0$ for the upper half plane and $\dim(\ker(-i-A^*)) = 0$ for the lower half plane) or they are contained in $\sigma(A)$. Since $\sigma(A)$ is closed, it can therefore either be empty, equal to the closed upper half plane, to the closed lower half plane, to the complex plane or a subset of the real line.

iii) Suppose $A = A^*$ and $\ker(i-A) \neq \{0\}$, that is $\dim(\ker(\overline{z}-A^*)) \neq 0$ for $z = -i$. Then, there exists $0 \neq \psi \in D(A)$ s.t.

$$i\langle\psi,\psi\rangle_{\mathcal{H}} = \langle\psi, A\psi\rangle_{\mathcal{H}} = \langle A\psi,\psi\rangle_{\mathcal{H}} = -i\langle\psi,\psi\rangle_{\mathcal{H}}$$

This implies $\psi = 0$, a contradiction. Arguing in the same way for $\ker(i+A)$, we conlude from *i)*, *ii)* and $A = A^*$ that $\sigma(A) \subset \mathbb{R}$.

Conversely, if $\sigma(A) \subset \mathbb{R}$, *i)* and *ii)* imply that $\operatorname{ran}(\pm i - A) = \mathcal{H}$. Let $\psi \in D(A^*)$ and choose $\xi \in D(A)$ s.t. $(i-A^*)\psi = (i-A)\xi$. Since $\xi \in D(A) \subset D(A^*)$, we have $(\psi-\xi) \in D(A^*)$ s.t.

$$(i-A^*)(\psi-\xi) = 0$$

This means that $(\psi-\xi) \in \ker(i-A^*) = \operatorname{ran}(-i-A)^{\perp} = \{0\}$, i.e. $\xi = \psi \in D(A)$. □

Corollary 2.1. *Let $A : D(A) \to \mathcal{H}$ be self-adjoint and s.t. $\langle\varphi, A\varphi\rangle_{\mathcal{H}} \geq 0$ for all $\varphi \in D(A)$. Then $\sigma(A) \subset [0,\infty)$.*

Proof. For $x \in (-\infty, 0)$, the positivity implies that

$$\|(x-A)\varphi\|_{\mathcal{H}}^2 = \|A\varphi\|_{\mathcal{H}}^2 - 2x\langle\varphi, A\varphi\rangle_{\mathcal{H}} + x^2\|\varphi\|_{\mathcal{H}}^2 \geq x^2\|\varphi\|_{\mathcal{H}}^2$$

for all $\varphi \in D(A)$. Arguing as in Theorem 2.3, we deduce that $\dim(\ker((z-A^*))$ is constant for all $z \in \mathbb{C}\setminus[0,\infty)$. Since A is self-adjoint, we conclude $\dim(\ker((z-A^*)) = 0$ for all $z \in \mathbb{C}\setminus[0,\infty)$ such that $\sigma(A) \subset [0,\infty)$. □

Corollary 2.2. *Let $A : D(A) \to \mathcal{H}$ be symmetric. Then, the following is equivalent:*

i) A is essentially self-adjoint.

ii) $\ker(A^* \pm i) = \{0\}$.

iii) $\operatorname{ran}(A \pm i)$ is dense.

Proof. We apply Theorem 2.3 and use that $\operatorname{ran}(\overline{A} \pm i) = \overline{\operatorname{ran}(A \pm i)}$. To prove this last fact, recall that $\varphi \in D(\overline{A})$ if and only if there exists a sequence $(\varphi_n)_{n\in\mathbb{N}}$ such that $\varphi_n \in D(A)$ for all $n \in \mathbb{N}$, $\lim_{n\to\infty} \varphi_n = \varphi$ and $\lim_{n\to\infty} A\varphi_n$ exists. In particular, if $\psi \in \operatorname{ran}(\overline{A}\pm i)$, then $\psi = (\overline{A}\pm i)\varphi$ for some $\varphi \in D(\overline{A})$ so that $\psi \in \overline{\operatorname{ran}(A \pm i)}$. Conversely, if $\psi \in \overline{\operatorname{ran}(A \pm i)}$, we know that $\psi = \lim_{n\to\infty}(\overline{A}\pm i)\varphi_n$ for suitable $\varphi_n \in D(A)$. By (2.3), $(\varphi_n)_{n\in\mathbb{N}}$ converges to some $\varphi \in \mathcal{H}$ and thus $\varphi \in D(\overline{A})$ so that $\psi \in \operatorname{ran}(\overline{A} \pm i)$. □

2.3 Examples of Self-Adjoint Operators and Self-Adjointness Criteria

In this section, we give several basic examples of self-adjoint operators that play an important role in quantum mechanics.

Proposition 2.1 (Multiplication Operators)**.** *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and let $f : \Omega \to \mathbb{R}$ be a real-valued, measurable function which is finite for a.e. $x \in \Omega$. Define $A_f : D(A_f) \to L^2(\Omega, \mathcal{A}, \mu)$ as the multiplication operator $A_f(\varphi) = f\varphi$ on the domain $D(A_f) = \{\psi \in L^2(\Omega, \mathcal{A}, \mu) : f\psi \in L^2(\Omega, \mathcal{A}, \mu)\}$. Then A_f is self-adjoint.*

Proof. Let $\psi \in L^2(\Omega, \mathcal{A}, \mu)$. Using the Dominated Convergence Theorem, we see that the sequence $(\psi\chi_{\{|f|\leq n\}})_{n\in\mathbb{N}}$ with $\psi\chi_{\{|f|\leq n\}} \in D(A_f)$ for all $n \in \mathbb{N}$, satisfies

$$\lim_{n\to\infty} \|\psi - \psi\chi_{\{|f|\leq n\}}\|_2 = 0$$

Hence, $D(A_f) \subset L^2(\Omega, \mathcal{A}, \mu)$ is dense. Since f is real-valued, it is clear that A_f is symmetric. A_f is also closed, since $\varphi_n \to \varphi \in L^2(\Omega, \mathcal{A}, \mu)$ and $A_f(\varphi_n) \to \psi \in L^2(\Omega, \mathcal{A}, \mu)$ as $n \to \infty$ imply $\psi(x) = f(x)\varphi(x)$ for *a.e.* $x \in \Omega$ by choosing suitable pointwise *a.e.* convergent subsequences. In particular, $\varphi \in D(A_f)$ and $\psi = A_f(\varphi) = f\varphi$. Finally, $(f+i)^{-1} : L^2(\Omega, \mathcal{A}, \mu) \to D(A_f)$ and $(f-i)^{-1} : L^2(\Omega, \mathcal{A}, \mu) \to D(A_f)$, defined pointwise *a.e.* in Ω as multiplication operators, are well-defined and bounded which follows from

$$\|(f+i)^{-1}\|_\infty \leq 1, \|(f-i)^{-1}\|_\infty \leq 1$$

Thus, $\{\pm i\} \in \rho(A_f)$ s.t. $\sigma(A) \subset \mathbb{R}$ showing that A_f is self-adjoint, by Theorem 2.3. □

Example 2.15. *The Laplace operator $\Delta : H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is self-adjoint. Denoting by $\mathfrak{F} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ the $L^2(\mathbb{R}^d)$-Fourier transform, that is*

$$(\mathfrak{F}(f))(p) = \widehat{f}(p) = \int_{\mathbb{R}^d} dx\, e^{-2\pi i p\cdot x} f(x),\ \forall\, p \in \mathbb{R}^d,$$

the Laplacian is in fact unitarily equivalent to the multiplication operator $\mathfrak{F}\,\Delta\,\mathfrak{F}^{-1} : \mathfrak{F}(H^2(\mathbb{R}^d)) \to L^2(\mathbb{R}^d)$ defined by

$$(\mathfrak{F}\,\Delta\,\mathfrak{F}^{-1}\widehat{\psi})(p) = -4\pi^2|p|^2\widehat{\psi}(p),\ \textit{for a.e. } p \in \mathbb{R}^d$$

Moreover, Δ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^d)$. To see this, let $\varphi \in D\big(\overline{\Delta_{|C_c^\infty}}\big)$. By definition of the closure, this implies that there exists a sequence $(\varphi_n)_{n\in\mathbb{N}}$ in $C_c^\infty(\mathbb{R}^d)$ and $\psi \in L^2(\mathbb{R}^d)$ such that

$$\lim_{n\to\infty} \|\varphi - \varphi_n\|_2 = \lim_{n\to\infty} \|\psi - \Delta\varphi_n\|_2 = 0$$

We conclude from the Fourier characterization of $H^2(\mathbb{R}^d)$ *that* $(\varphi_n)_{n\in\mathbb{N}}$ *is a Cauchy sequence in* $H^2(\mathbb{R}^d)$*. By the completeness of* $H^2(\mathbb{R}^d)$*, this implies that* $\varphi \in H^2(\mathbb{R}^d)$ *and* $\psi = \Delta\varphi$*, i.e.* $\overline{\Delta_{|C_c^\infty}} \subset \Delta$*. Since* $C_c^\infty(\mathbb{R}^d) \subset H^2(\mathbb{R}^d)$ *is dense, it is also clear that* $\Delta \subset \overline{\Delta_{|C_c^\infty}}$*, so that altogether* $\overline{\Delta_{|C_c^\infty}} = \Delta$*.*

Notice that in the last example we have used that self-adjointness is preserved under unitary transformations: if $A : D(A) \to \mathcal{H}$ is self-adjoint on the Hilbert space $\mathcal{H}$ and if $U : \mathcal{H} \to \widetilde{\mathcal{H}}$ is a unitary map to the Hilbert space $\widetilde{\mathcal{H}}$, then $UAU^{-1} : U(D(A)) \to \widetilde{\mathcal{H}}$ is also self-adjoint. In fact, the spectrum $\sigma(A)$ of a linear operator A is invariant under unitary conjugation, because $R_z(UAU^{-1}) = UR_z(A)U^{-1}$ for all $z \in \rho(A)$.

Example 2.16. *Consider the space* $L^2([0,1]^d)$ *for which* $\{x \mapsto e^{2\pi i p x} : p \in \mathbb{Z}^d\}$ *is a complete orthonormal basis. The discrete Fourier transform* $\mathfrak{F}_d : L^2([0,1]^d) \to \ell^2(\mathbb{Z}^d)$ *is a unitary map and we can define the Laplacian with periodic boundary conditions* $\Delta : D(\Delta) \to L^2([0,1]^d)$ *as the Fourier multiplier*

$$(\mathfrak{F}_d\, \Delta\, \mathfrak{F}_d^{-1} \widehat{f})_p = -4\pi^2 |p|^2 \widehat{f}_p,\ \forall p \in \mathbb{Z}^d,$$

with domain $D(\Delta) = \mathfrak{F}_d^{-1}\big\{\widehat{f} = (\widehat{f}_p)_{p\in\mathbb{Z}^d} \in \ell^2(\mathbb{Z}^d) : \sum_{p\in\mathbb{Z}^d} |p|^4 |\widehat{f}_p|^2 < \infty\big\}$*. We can identify the operator with the Laplacian* Δ *on* $L^2(\mathbb{T}^d)$*, where* $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$ *denotes the* d*-dimensional unit torus.*

In quantum mechanics, a special role is given to the Hamilton operator, or simply Hamiltonian, which is a self-adjoint operator describing the energy of the system. For many systems, it is essentially given by the sum of an operator describing the kinetic energy of the particles and an operator describing the interaction energies among the particles. The kinetic energy is described by (a self-adjoint realization of) the Laplace operator while the interaction energy is described by a multiplication operator. To ensure the sum of such operators to be self-adjoint, we present two basic results: the Kato-Rellich Theorem and Kato's inequality.

The Kato-Rellich Theorem shows that self-adjointness is stable under suitable perturbations, as defined as follows. Let $A : D(A) \to \mathcal{H}$ and $B : D(B) \to \mathcal{H}$ be densely defined linear operators on some Hilbert space $\mathcal{H}$. We say that B is A-bounded if

$$\begin{aligned} &i)\ D(A) \subset D(B) \\ &ii)\ \exists\, a, b \in \mathbb{R} \text{ s.t. } \forall\, \varphi \in D(A) :\ \|B\varphi\|_{\mathcal{H}} \le a\|A\varphi\|_{\mathcal{H}} + b\|\varphi\|_{\mathcal{H}} \end{aligned} \tag{2.5}$$

Notice that the assumption (2.5) *i)* is quite reasonable if B is supposed to be a perturbation of A: if $A\psi$ makes sense, $B\psi$ should certainly make sense as well.

The infimum over all $a \in \mathbb{R}$ such that (2.5) *ii)* holds true is called the relative bound of B with respect to A. If the relative bound is equal to zero, we say that B is infinitesimally small with respect to A.

Theorem 2.4 (Kato-Rellich Theorem)**.** *Assume that* $A : D(A) \to \mathcal{H}$ *is self-adjoint, that* $B : D(B) \to \mathcal{H}$ *is symmetric and that* B *is* A*-bounded with relative bound* $a_0 < 1$*. Then* $A + B$ *is self-adjoint on* $D(A)$ *and essentially self-adjoint on any core of* A*.*

Proof. $A + B : D(A) \to \mathcal{H}$ is well-defined ($D(A) \subset D(B)$), it is clearly symmetric and it is closed. For this last fact, note that if $(\varphi_n)_{n\in\mathbb{N}}$ converges to $\varphi \in \mathcal{H}$ and if $((A+B)\varphi_n)_{n\in\mathbb{N}}$ converges, then also $(A\varphi_n)_{n\in\mathbb{N}}$ converges, because

$$\|(A+B)\psi\| \geq \|A\psi\| - \|B\psi\| \geq (1-a_0)\|A\psi\| - b\|\psi\|$$

for all $\psi \in D(A)$. Since A is closed, this implies $\varphi \in D(A)$ and $\lim_{n\to\infty} A\varphi_n = A\varphi$. Moreover, since B is A-bounded, we also find that $\lim_{n\to\infty} B\varphi_n = B\varphi$. Combining this, we conclude that $\varphi \in D(A)$ and $\lim_{n\to\infty}(A+B)\varphi_n = (A+B)\varphi$, that is, $A+B$ is closed.

Now we can apply Theorem 2.3. To show that $A+B$ is self-adjoint, it is enough to prove that $\operatorname{ran}(A+B+i\mu) = \mathcal{H}$ for $\mu \in \mathbb{R}$ with $|\mu|$ sufficiently large. To this end, the perturbative idea is to rewrite

$$A + B + i\mu = \big(1 + B(A+i\mu)^{-1}\big)(A+i\mu) \tag{2.6}$$

and to show that $C = B(A+i\mu)^{-1}$ has operator norm less than one. As a consequence, $1 + C : \mathcal{H} \to \mathcal{H}$ is invertible: its inverse can be computed using the Neumann series

$$(1+C)^{-1} = \sum_{k=0}^{\infty} (-1)^k C^k$$

and, since $i\mu \in \rho(A)$, we conclude that $\operatorname{ran}(A+B+i\mu) = \mathcal{H}$.

So, let us prove that C has operator norm less than one if $|\mu|$ is sufficiently large. First of all, we have for all $\varphi \in D(A)$ that

$$\|(A+i\mu)\varphi\|_{\mathcal{H}}^2 = \|A\varphi\|_{\mathcal{H}}^2 + \mu^2\|\varphi\|_{\mathcal{H}}^2 \geq \|A\varphi\|_{\mathcal{H}}^2$$

This implies that $\|A(A+i\mu)^{-1}\|_{\mathcal{L}(\mathcal{H})} \leq 1$. From Theorem 2.3, we also know that $\|(A+i\mu)^{-1}\|_{\mathcal{L}(\mathcal{H})} \leq |\mu|^{-1}$. Hence, from the A-boundedness of B we find for some $a < 1$

$$\|B(A+i\mu)^{-1}\psi\|_{\mathcal{H}} \leq a\|A(A+i\mu)^{-1}\psi\|_{\mathcal{H}} + b\|(A+i\mu)^{-1}\psi\|_{\mathcal{H}} \leq \big(a + |\mu|^{-1}b\big)\|\psi\|_{\mathcal{H}}$$

for all $\psi \in \mathcal{H}$. If we choose $|\mu|$ sufficiently large, we obtain that $\|C\|_{\mathcal{L}(\mathcal{H})} < 1$.

The statement about the operator core can be proved in the same way. In this case, we apply Corollary 2.2 (with $\pm i$ replaced by $i\mu$ for $\mu \in \mathbb{R}$ and $|\mu|$ large enough). The essential self-adjointness of $(A+B)_{|D} : D \to \mathcal{H}$ then follows if $\operatorname{ran}((A+i\mu)(1+C^*)_{|D})$ is dense in $\mathcal{H}$ which is the case if $\operatorname{ran}((A+i\mu)_{|D})$ is dense, by invertibility of $1+C^* : \mathcal{H} \to \mathcal{H}$. But $A_{|D} : D \to \mathcal{H}$ is essentially self-adjoint (by assumption that D is a core for A) so that applying the corollary to A implies that $(A+B)_{|D} : D \to \mathcal{H}$ is essentially self-adjoint. □

Proposition 2.2. *Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ be real-valued. Then $-\Delta + V$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3)$ and self-adjoint on $H^2(\mathbb{R}^3)$.*

Proof. We apply Theorem 2.4 and view the potential V as a perturbation of $-\Delta$. Write $V = V_2 + V_\infty$, where $V_2 \in L^2(\mathbb{R}^3)$, $V_\infty \in L^\infty(\mathbb{R}^3)$, then for $\varphi \in C_c^\infty(\mathbb{R}^3)$, we bound

$$\|V\varphi\|_2 \leq \|V_2\|_2\|\varphi\|_\infty + \|V_\infty\|_\infty\|\varphi\|_2.$$

Applying the inverse Fourier transform and Cauchy-Schwarz, we estimate

$$\begin{aligned}\|\varphi\|_\infty \le \|\mathfrak{F}^{-1}(\varphi)\|_1 &\le \int_{|p|\ge\varepsilon^{-2}} dp\,\frac{1}{|p|^2}\,|p|^2\mathfrak{F}^{-1}(\varphi)(p) + C_\varepsilon\|\varphi\|_2\\ &\le \Big(\int_{|p|\ge\varepsilon^{-2}} dp\,\frac{1}{|p|^4}\Big)^{1/2}\Big(\int_{\mathbb{R}^3} dp\,|p|^4\big|\mathfrak{F}^{-1}(\varphi)(p)\big|^2\Big)^{1/2}\\ &\le C\varepsilon\|-\Delta\varphi\|_2 + C_\varepsilon\|\varphi\|_2\end{aligned}$$

for some universal constant $C>0$ and for all $\varepsilon>0$. By density of $C_c^\infty(\mathbb{R}^3)$, the previous inequality is also true on $H^2(\mathbb{R}^3)$ and the proposition follows from Theorem 2.4. The statement about essential self-adjointness follows from the fact that $-\Delta$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3)$. □

As a corollary, we conclude that $-\Delta - \frac{e^2}{|x|}$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3)$. This Schrödinger operator describes (after a change of variables to center of mass and relative coordinates) the hydrogen atom, consisting of one proton and one electron ($-e$ is interpreted as the charge of the electron). That the potential $x\mapsto |x|^{-1}$ is infinitesimally small with respect to $-\Delta$ can alternatively be seen through *Hardy's inequality.*

Lemma 2.3 (Hardy's inequality)**.** *For all $\varphi\in H^1(\mathbb{R}^d)$ and $d\ge 3$, we have that*

$$\big\||x|^{-1}\varphi\big\|_2 \le \frac{2}{d-2}\|\nabla\varphi\|_2.$$

Proof. We follow [47, Prop. 10.3]. Denote by $\widehat{p}=i\nabla$ and by $\widehat{x}$ multiplication by x in $\mathbb{R}^d$. It is an elementary computation to check the commutator identity

$$d|x|^{-2} = -i\big[|x|^{-1}\widehat{p}\,|x|^{-1},\widehat{x}\big] =: \sum_{j=1}^d \big[|x|^{-1}\partial_j|x|^{-1},x_j\big],$$

in $C_c^\infty(\mathbb{R}^3)$. Indeed, we obtain from $\partial_j|x|^{-1} = -|x|^{-3}x_j + |x|^{-1}\partial_j$ that

$$\begin{aligned}\big[|x|^{-1}\partial_j|x|^{-1},x_j\big] &= |x|^{-1}\big(-|x|^{-3}x_j+|x|^{-1}\partial_j\big)x_j - x_j|x|^{-1}\big(-|x|^{-3}x_j+|x|^{-1}\partial_j\big)\\ &= |x|^{-2}.\end{aligned}$$

This shows

$$\begin{aligned}d\||x|^{-1}\varphi\|_2^2 = d\langle\varphi,|x|^{-2}\varphi\rangle_2 &= \big\langle\varphi,-i\big[|x|^{-1}\widehat{p}\,|x|^{-1},\widehat{x}\big]\varphi\big\rangle_2\\ &= 2\,\mathrm{Im}\langle|x|^{-1}\widehat{p}\,|x|^{-1}\varphi,\widehat{x}\varphi\rangle_2\\ &= 2\,\mathrm{Im}\langle\widehat{p}\,\varphi,\widehat{x}|x|^{-2}\varphi\rangle_2 + 2\langle\varphi,|x|^{-2}\varphi\rangle_2,\end{aligned}$$

so that for all $\varphi\in C_c^\infty(\mathbb{R}^3)$, we have that

$$(d-2)\||x|^{-1}\varphi\|_2^2 = -2\,\mathrm{Im}\langle\widehat{p}\,\varphi,\widehat{x}\,|x|^{-2}\varphi\rangle_2.$$

The claim now follows by applying Cauchy-Schwarz on the r.h.s. of the last equation and by using the density of $C_c^\infty(\mathbb{R}^d)$ in $H^1(\mathbb{R}^d)$. □

Problem 2.6. *Use Hardy's inequality to prove that* $x \mapsto |x|^{-1}$ *is infinitesimally small with respect to* $-\Delta$ *in* $\mathbb{R}^3$.

Proposition 2.3. *Let* $v \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$*. Then the operator*

$$H_N = \sum_{i=1}^N (-\Delta_{x_i}) + \sum_{1\leq i<j\leq N} v(x_i - x_j)$$

is essentially self-adjoint on $C_c^\infty(\mathbb{R}^{3N})$ *and self-adjoint on* $H^2(\mathbb{R}^{3N})$.

Remark. *The Hamiltonian* H_N *defined in Theorem 2.3 describes a system of N particles that move in* $\mathbb{R}^3$ *and interact through the pair potential* $v \in L^2(\mathbb{R}^3)+L^\infty(\mathbb{R}^3)$*. By* $(-\Delta_{x_i})$*, we denote the Laplacian w.r.t. the i-th coordinate* $x_i \in \mathbb{R}^3$*,* $i = 1, \dots, N$*. It describes the kinetic energy of the i-th particle.*

Proof of Proposition 2.3. As before, we apply Theorem 2.4 by viewing the interaction operator as a perturbation of the Laplacian. Choose w.l.o.g. $i = 1, j = 2$ and let $v = v_1 + v_2$ where $v_1 \in L^2(\mathbb{R}^3)$, $v_2 \in L^\infty(\mathbb{R}^3)$. For any $\varphi \in H^2(\mathbb{R}^{3N})$, we certainly have[2]

$$\|v_2(x_1 - x_2)\varphi\|_2 \leq \|v_2\|_\infty \|\varphi\|_2$$

Hence, let us focus on bounding $v_1 \in L^2(\mathbb{R}^3)$ in terms of the Laplacian. Denoting by $X_{N-2} = (x_3, x_4, \dots, x_N)$, we proceed as above and use Fubini so that

$$\begin{aligned}
\|v_1(x_1 - x_2)\varphi\|_2^2 &\leq \int_{\mathbb{R}^{3(N-1)}} \|v_1(. - x_2)\|_{L^2(\mathbb{R}^3)} \|\varphi(\cdot, x_2, X_{N-2})\|^2_{L^\infty(\mathbb{R}^3)} \, dx_2 dX_{N-2} \\
&\leq \varepsilon \int_{\mathbb{R}^{3N}} |(-\Delta_{x_1})\varphi(x_1, x_2, X_{N-2})|^2 \, dx_1 dx_2 dX_{N-2} \\
&\quad + C_\varepsilon \int_{\mathbb{R}^{3N}} |\varphi(x_1, x_2, X_{N-2})|^2 \, dx_1 dx_2 dX_{N-2} \\
&\leq \varepsilon \int_{\mathbb{R}^{3N}} \Big| \sum_{i=1}^N (-\Delta_{x_i})\varphi(x) \Big|^2 \, dx + C_\varepsilon \|\varphi\|_2^2
\end{aligned}$$

Since $\varepsilon > 0$ can be chosen arbitrarily small, the claim follows from Theorem 2.4. □

Hamiltonians as in Proposition 2.3 describe particles that move in all of $\mathbb{R}^3$ and interact via some pair interaction. When we study the energy of a system of bosons, we consider instead Hamiltonians which describe particles that are trapped in a finite region in $\mathbb{R}^3$. This can be modelled by adding an external potential $V_{\text{ext}} \in L^\infty_{\text{loc}}(\mathbb{R}^3)$ with $V_{\text{ext}}(x) \to \infty$ as $|x| \to \infty$. The growth of V_{ext} at infinity prevents that particles escape to infinity so that they are effectively trapped in a finite region in $\mathbb{R}^3$. To prove the self-adjointness of Hamilton operators with growing potentials, we use *Kato's inequality*

[2] For notational simplicity, we denote by $v(x_i - x_j)$ the multiplication operator which is defined *a.e.* in $\mathbb{R}^{3N}$ as the multiplication by $v(x_i - x_j)$ at $x = (x_1, \dots, x_i, \dots, x_j, \dots, x_N) \in \mathbb{R}^{3N}$.

which is a suitable bound interpreted in distributional sense. Before discussing this result and its consequences, let us recall a few basics on distributions. For concreteness, we describe a hands-on approach as discussed for example in [66, 40].

A large part of analysis is devoted to solving partial differential equations. Given a PDE, one may ask for example if it admits a regular solution, but in general one can not simply integrate a PDE. It is usually not even obvious if a solution exists and what its optimal regularity might be. The question then arises where, i.e. in what kind of function space, we should start to look for a solution - and with minimal assumptions, we might want to look in a space of rather rough objects whose regularity properties can then be analyzed once a solution is found. Distributions are a certain class of rough objects and they generalize the concept of a classical function.

Let Ω be some open subset in $\mathbb{R}^d$, then we denote by $\mathcal{D}(\Omega) = \mathcal{D} = C_c^\infty(\Omega)$ the set of test functions (unless stated explicitly, the choice of base space Ω will be clear from context). In $\mathcal{D}$, we define the following notion of convergence: a sequence $(\varphi_n)_{n\in\mathbb{N}}$, such that $\varphi_n \in \mathcal{D}$ for all $n \in \mathbb{N}$, converges to $\varphi \in \mathcal{D}$ in $\mathcal{D}$ if and only

$$
\begin{aligned}
&i)\ \exists\, K \subset \Omega \text{ compact such that } \operatorname{supp}(\varphi_n) \subset K \ \forall\, n \in \mathbb{N},\\
&ii)\ \lim_{n\to\infty} \sup_{x\in\Omega} |\partial^\alpha(\varphi_n - \varphi)| = \lim_{n\to\infty} \|\partial^\alpha(\varphi_n - \varphi)\|_\infty = 0 \ \ \forall\, \alpha \in \mathbb{N}_0^d.
\end{aligned}
$$

A distribution T is a linear functional $T : \mathcal{D} \to \mathbb{C}$ which is sequentially continuous in the sense that $\lim_{n\to\infty} T(\varphi_n) = T(\varphi)$ whenever $\lim_{n\to\infty} \varphi_n = \varphi$ in $\mathcal{D}$. It is straightforward to check that the set of distributions with the usual addition and scalar multiplication forms a vector space. This space is denoted in the sequel by[3] $\mathcal{D}'(\Omega)$. We say that a sequence of distributions $(T_n)_{n\in\mathbb{N}}$, such that $T_n \in \mathcal{D}'$ for all $n \in \mathbb{N}$, converges weakly to $T \in \mathcal{D}'$ if and only if $\lim_{n\to\infty} T_n(\varphi) = T(\varphi)$ for every $\varphi \in \mathcal{D}$.

Example 2.17. *Let $f \in L^p_{loc}(\Omega)$, then f determines the distribution*

$$T_f(\varphi) = \int_\Omega dx\, f(x)\varphi(x).$$

Recall that functions are uniquely determined by the associated distributions: if $T_f(\varphi) = T_g(\varphi)$ for all $\varphi \in \mathcal{D}$, then $f = g$ almost surely by standard measure theoretic arguments.

Example 2.18. *Let μ be a Radon measure on Ω, then μ determines the distribution*

$$T_\mu(\varphi) = \int_\Omega \mu(dx)\, \varphi(x).$$

The previous example shows that distributions naturally generalize the concept of a function: although some object may not correspond to a classical function, it may still have a natural action on sufficiently nice test functions, like a Radon measure.

[3]This notation suggests that $\mathcal{D}'$ is the topological dual space of $\mathcal{D}$ equipped with a suitable topology that is consistent with the notion of sequential continuity defined above. This can in fact be made precise; see below for a short discussion on this.

A prominent example from physics, which models e.g. point masses or point charges, is the *Dirac* δ distribution $\delta_x : \mathcal{D} \to \mathbb{C}$ centered at $x \in \Omega$, which is defined by

$$\delta_x(\varphi) = \varphi(x).$$

Informally, one may write $\delta_x(\varphi) = \int_\Omega dx\, \delta_x(y)\varphi(y)$ and think of δ_x to correspond to a function which is infinite at $x \in \Omega$ and zero else. Although mathematically, a δ_x function in this sense does not exist, the intuition it provides is nevertheless quite useful.

Problem 2.7. *Show that there exists no function $f \in L^1_{loc}(\Omega)$ such that $T_f = \delta_x$.*

Generalizing the concept of a function by duality (that is, f vs. T_f), one can also attempt to generalize basic properties of functions by duality, like e.g. differentiation. If $T : \mathcal{D} \to \mathbb{C}$ is a distribution, its derivative $\partial^\alpha T : \mathcal{D} \to \mathbb{C}$, for $\alpha \in \mathbb{N}_0^d$, is the distribution (*exercise*), defined by

$$\partial^\alpha T(\varphi) = (-1)^{|\alpha|} T(\partial^\alpha \varphi) \quad (\partial^\alpha = \partial_1^{\alpha_1} \ldots \partial_d^{\alpha_d}).$$

This is consistent with the usual integration by parts formula for functions in $\mathcal{D}$. Defined in this weak sense, every distribution is smooth and has derivatives of all orders.

Example 2.19. *Let $h(x) = \chi_{|[0,\infty)}$ denote the Heaviside function in $\mathbb{R}$. Then*

$$\partial_x T_h(\varphi) = -\int_0^\infty \partial_x \varphi(x) dx = \varphi(0) = \delta(\varphi),$$

that is $\partial_x T_h = \delta = \delta_0$ (compare this with the interpretation of δ as an infinite peak centered at zero, mentioned above).

Problem 2.8. *Suppose that $f \in C^k(\Omega)$. Show that $\partial^\alpha T_f = T_{\partial^\alpha f}$ for every $\alpha \in \mathbb{N}_0^d$ with $|\alpha| \leq k$ so that in case of a regular function its distributional derivatives coincide with its classical derivatives.*

Using duality arguments as above, there are many further properties which can be generalized naturally from classical to generalized functions, e.g. the concept of the convolution of a distribution with a test function $\psi \in \mathcal{D}$ (see [66, 40] for further properties). For simplicity of notation, let us consider $\Omega = \mathbb{R}^d$ for the remainder of this discussion. We can interpret $(T * \psi)$ of $T \in \mathcal{D}'$ with $\psi \in \mathcal{D}$ in two ways: setting

$$\psi_y(x) = \psi(x - y) \quad \text{and} \quad \psi_R(x) = \psi(-x) \ \forall\, \psi \in C^\infty(\mathbb{R}^d),$$

we can define $(T * \psi) \in C^\infty(\mathbb{R}^d)$ on the one hand as the smooth function $x \mapsto T((\psi_R)_x)$ and, on the other hand, we can interpret $(T * \psi) \in \mathcal{D}'$ as the distribution defined by $(T * \psi)(\varphi) = T(\psi_R * \varphi)$. Note that we assume $\psi \in \mathcal{D}$ for both objects to be well-defined. That the two notions coincide, in the sense of distributions, follows from the next lemma.

Lemma 2.4. *Let $T \in \mathcal{D}'$ and $\varphi \in \mathcal{D}$. Then, $\mathbb{R}^d \ni x \mapsto T(\varphi_x) \in C^\infty(\mathbb{R}^d)$ with*

$$\partial_x^\alpha T(\varphi_x) = (-1)^{|\alpha|} T\big((\partial^\alpha \varphi)_x\big) = (\partial^\alpha T)(\varphi_x).$$

Moreover, if $\psi \in \mathcal{D}$ we have that

$$\int_{\mathbb{R}^d} dx\, T(\varphi_x)\psi(x) = T(\psi * \varphi). \tag{2.7}$$

Proof. Let us prove that $x \mapsto T(\varphi_x) \in C^1(\mathbb{R}^d)$; the smoothness follows with analogous arguments and induction (*exercise*). Let us start with continuity. Suppose that $h_n \to 0$ as $n \to \infty$. Since $\varphi \in \mathcal{D}$, we have for every $\alpha \in \mathbb{N}_0^d$ and $\epsilon > 0$ that there exists a constant $C_\alpha > 0$ such that for $n \geq N_\epsilon$ so that $|h_n| \leq \epsilon$, we have that

$$\sup_{y \in \mathbb{R}^d} |\partial^\alpha \varphi_x(y) - \partial^\alpha \varphi_{x+h_n}(y)| \leq C_\alpha \epsilon, \;\; \forall\, n \geq N_\epsilon.$$

Combining this with the fact that for a suitable compact set $K \subset \mathbb{R}^d$, we have

$$\operatorname{supp}(\varphi_x) \cup \bigcup_{n\in\mathbb{N}} \operatorname{supp}(\varphi_{x+h_n}) \subset K,$$

we conclude that $\lim_{n\to\infty} \varphi_{x+h_n} = \varphi_x$ in $\mathcal{D}$. Since $T \in \mathcal{D}'$, we get that

$$\lim_{n\to\infty} T(\varphi_{x+h_n}) = T(\varphi_x)$$

and since $x \in \mathbb{R}^d$ and $(h_n)_{n\in\mathbb{N}}$were arbitrary, this shows that $x \mapsto T(\varphi_x) \in C(\mathbb{R}^d)$.

To prove continuous differentiability, we argue very similarly, observing in this case (with analogous notation as above) that we have

$$\sup_{y\in\mathbb{R}^d} \Big|\partial^\alpha\Big(|h_n|^{-1}\big(\varphi_{x+h_n}(y) - \varphi_x(y)\big) - (-1)(\nabla\varphi)_x(y)\cdot |h_n|^{-1} h_n\Big)\Big| \leq C_\alpha \epsilon, \;\; \forall\, n \geq N_\epsilon.$$

Arguing as above, this implies that

$$\lim_{h\to 0} |h|^{-1} \Big| T(\varphi_{x+h}) - T(\varphi_x) - \sum_{i=1}^d T(-(\partial_i\varphi)_x) h_i \Big| = 0,$$

i.e. $x \mapsto T(\varphi_x)$ is differentiable with derivatives in $C(\mathbb{R}^d)$, given by

$$\partial_{x_i} T(\varphi_x) = (\partial_i T)(\varphi_x).$$

In order to prove (2.7), we use an approximation argument. By the first part and the fact that $\operatorname{supp}(\varphi) \subset \mathbb{R}^d$ is compact, the integrand $x \mapsto T(\varphi_x)\psi(x)$ on the l.h.s. in (2.7) is a $C_c^\infty(\mathbb{R}^d)$ function. Hence, we can approximate it by a Riemann sum

$$\int_{\mathbb{R}^d} dx\, T(\varphi_x)\psi(x) = \lim_{N\to\infty} \Delta_N \sum_{j=1}^N T(\varphi_{x_j})\psi(x_j) = \lim_{N\to\infty} T\Big(\Delta_N \sum_{j=1}^N \varphi(.-x_j)\psi(x_j)\Big)$$

for suitable lattice points $(x_j)_{j=1}^N$ with mesh size $\Delta_N \to 0$ as $N \to \infty$. Similarly, we have the uniform approximations

$$\lim_{N\to\infty} \sup_{x\in\mathbb{R}^d} \left| \partial^\alpha \left(\Delta_N \sum_{j=1}^N \varphi(x - x_j)\psi(x_j) - (\psi * \varphi)(x) \right) \right| = 0$$

for every multi-index $\alpha \in \mathbb{N}_0^d$. This implies that $\psi_N = \Delta_N \sum_{j=1}^N \varphi(\cdot - x_j)\psi(x_j)$ converges to $(\psi*\varphi)$ in $\mathcal{D}$, arguing similarly as before. Combining this with $T \in \mathcal{D}'$, we get (2.7). $\square$

Problem 2.9. *Extend* (2.7) *to* $\psi \in L^1(\mathbb{R}^d)$*, assuming supp*$(\psi) \subset \mathbb{R}^d$ *to be compact.*

Proposition 2.4 (Fundamental Theorem of Calculus for Distributions.)**.** *Assume that* $T \in \mathcal{D}'(\mathbb{R}^d) = \mathcal{D}'$ *and let* $\varphi \in \mathcal{D}$*. Then we have that*

$$T(\varphi_y) - T(\varphi) = \int_0^1 dt \sum_{j=1}^d y_j (\partial_j T)(\varphi_{ty}) = \int_0^1 dt\, y \cdot (\nabla T)(\varphi_{ty}). \tag{2.8}$$

Proof. Let us denote the function defined through the r.h.s. in (2.8) by $y \mapsto G(y)$. By Lemma 2.4, the map $x \mapsto (\nabla T)(\varphi_x) \in C^\infty(\mathbb{R}^d)$ with $\partial_{x_j}(\nabla T)(\varphi_x) = -(\nabla T)((\partial_j\varphi)_x)$. Using the smoothness and the fact that we integrate over a compact interval, we compute the derivative of G by interchanging integration with differentiation and obtain that

$$\begin{aligned}
\partial_i G(y) &= -\int_0^1 dt\, t(\nabla T)((\partial_i\varphi)_{ty}) \cdot y + \int_0^1 dt\, (\partial_i T)(\varphi_{ty}) \\
&= -\int_0^1 dt \sum_{j=1}^d t y_j (\partial_i T)((\partial_j\varphi)_{ty}) + \int_0^1 dt\, (\partial_i T)(\varphi_{ty}) \\
&= \int_0^1 dt\, t\, \partial_t \Big((\partial_i T)(\varphi_{ty}) \Big) + \int_0^1 dt\, (\partial_i T)(\varphi_{ty}) = (\partial_i T)(\varphi_y),
\end{aligned}$$

where the second to last step follows with similar arguments as above (*exercise*) and the last step follows from integration by parts. Finally, the function

$$y \mapsto \widetilde{G}(y) = T(\varphi_y) - T(\varphi) \in C^\infty(\mathbb{R}^d)$$

has the same derivatives as G and it follows with $G(0) = \widetilde{G}(0) = 0$ that $G = \widetilde{G}$. $\square$

Problem 2.10. *Assume that* $f \in W^{1,1}_{loc}(\mathbb{R}^d)$*. Prove that for every* $y \in \mathbb{R}^d$*, we have*

$$f(x+y) = f(x) + \int_0^1 dt\, y \cdot \nabla f(x+ty)$$

for almost every $x \in \mathbb{R}^d$*.*

Recall from Problem 2.8 that the distributional derivatives of smooth functions correspond to their classical derivatives. We can now also show that if a distribution has continuous derivatives, it corresponds to a classical, continuously differentiable function.

Lemma 2.5. *Suppose that $T \in \mathcal{D}'$ is such that $g_i = \partial_i T \in \mathcal{D}'$ can be identified with $g_i \in C(\mathbb{R}^d)$ (in the usual distributional sense). Then $T \in C^1(\mathbb{R}^d)$ and its classical derivatives $\partial_i T$ are equal to $\partial_i T = g_i$.*

Proof. Pick $\varphi \in \mathcal{D}$. By Proposition 2.4 and Fubini, we know that

$$\begin{aligned}
T(\varphi_y) - T(\varphi) &= \int_0^1 dt \sum_{j=1}^d y_j (\partial_j T)(\varphi_{ty}) \\
&= \int_0^1 dt \sum_{j=1}^d y_j \Big(\int_{\mathbb{R}^d} dx \, g_j(x) \varphi(x - ty) \Big) \\
&= \int_{\mathbb{R}^d} dx \left(\int_0^1 dt \sum_{j=1}^d y_j g_j(x + ty) \right) \varphi(x).
\end{aligned}$$

Now, pick some $\psi \in \mathcal{D}$ with $\int_{\mathbb{R}^d} dx \, \psi(x) = 1$, then the previous identity implies that

$$\begin{aligned}
T(\varphi) &= \int_{\mathbb{R}^d} dy \, \psi(y) T(\varphi_y) - \int_{\mathbb{R}^d} dy \psi(y) \Big(\int_{\mathbb{R}^d} dx \left(\int_0^1 dt \sum_{j=1}^d y_j g_j(x + ty) \right) \varphi(x) \Big) \\
&= T(\psi * \varphi) - \int_{\mathbb{R}^d} dx \left(\int_{\mathbb{R}^d} dy \int_0^1 dt \, \psi(y) \sum_{j=1}^d y_j g_j(x + ty) \right) \varphi(x) \\
&= \int_{\mathbb{R}^d} dx \left(T(\psi_x) - \sum_{j=1}^d \int_{\mathbb{R}^d} dy \, \psi(y) \int_0^1 dt \, y_j g_j(x + ty) \right) \varphi(x),
\end{aligned}$$

representing T as an explicit function denoted in the sequel by $f \in C(\mathbb{R}^d)$.

Now, recalling that $\partial_{x_i} T(\psi_x) = (\partial_i T)(\psi_x)$ in classical sense and

$$\partial_j g_i = (\partial_i \partial_j T) = \partial_i g_j$$

in distributional sense, we get

$$\begin{aligned}
\partial_{x_i} \sum_{j=1}^d \int_0^1 dt \, y_j g_j(x + ty) &= \sum_{j=1}^d \int_0^1 dt \, y_j (\partial_i g_j)(x + ty) \\
&= \int_0^1 dt \, y \cdot (\nabla g_i)(x + ty) = g_i(x + y) - g_i(x)
\end{aligned}$$

and consequently (*exercise*) with $\partial_i T = g_i$ that in the sense of distributions, we have

$$\partial_{x_i} \left(T(\psi_x) - \sum_{j=1}^d \int_{\mathbb{R}^d} dy \, \psi(y) \int_0^1 dt \, y_j g_j(x + ty) \right) = g_i(x).$$

Finally, using the local integrability of f and the weak derivatives g_i, we may apply Problem 2.10 that shows for every $y \in \mathbb{R}^d$ that

$$f(x+y) = f(x) + \sum_{j=1}^{d} \int_0^1 y_j g_j(x+ty) = f(x) + \sum_{j=1}^{d} y_j g_j(x) + o(|y|)$$

almost surely in $x \in \mathbb{R}^d$ and hence, by continuity, for all $x \in \mathbb{R}^d$. Here, we used in the last step the continuity of the $g_i \in C(\mathbb{R}^d)$. By definition of differentiability, this shows that $f \in C^1(\mathbb{R}^d)$ with (classical) partial derivatives $\partial_i f = g_i$. $\square$

Problem 2.11. *Let $T \in \mathcal{D}'$ with $\partial_i T = 0$ for all $i = 1, \ldots, N$. Prove that*

$$T(\varphi) = C \int_{\mathbb{R}^d} dx\, \varphi(x)$$

for some $C \in \mathbb{R}$ and for all $\varphi \in \mathcal{D}$.

Finally, let us introduce the space of tempered distributions and their distributional Fourier transforms. As before, we might in a first attempt define the Fourier transform of $T \in \mathcal{D}'$ by duality, i.e. $\widehat{T}(\varphi) = T(\widehat{\varphi})$. However, here we encounter the problem that $\widehat{\varphi}$ need not be an element in $\mathcal{D}$ so that $\widehat{T}$ is ill-defined in $\mathcal{D}$. To resolve this problem, we may enlarge the space of test functions (i.e. we consider a smaller, more regular set of distributions) to the well-known space (see e.g. [55]) of rapidly decaying functions $\mathcal{S}(\mathbb{R}^d)$ - the Schwartz functions - which is defined as the space

$$\mathcal{S}(\mathbb{R}^d) = \mathcal{S} = \Big\{ \varphi \in C^\infty(\mathbb{R}^d) : |\varphi|_{\alpha,\beta} = \sup_{x \in \mathbb{R}^d} |x^\alpha \partial^\beta \varphi(x)| < \infty \quad \forall\, \alpha, \beta \in \mathbb{N}_0^d \Big\}.$$

It is well-known from basic Fourier theory that $\widehat{\varphi} \in \mathcal{S}$ whenever $\varphi \in \mathcal{S}$, that the Fourier inversion formula holds in $\mathcal{S}$ and that $\|\varphi\|_2 = \|\widehat{\varphi}\|_2$ for all $\varphi \in \mathcal{S}$. We say that a sequence $(\varphi_n)_{n \in \mathbb{N}}$, such that $\varphi_n \in \mathcal{S}$ for all $n \in \mathbb{N}$, converges to $\varphi \in \mathcal{S}$ in $\mathcal{S}$ if and only if

$$\lim_{n \to \infty} |\varphi - \varphi_n|_{\alpha,\beta} = 0, \;\; \forall\, \alpha, \beta \in \mathbb{N}_0^d.$$

We denote by $\mathcal{S}'(\mathbb{R}^d) = \mathcal{S}'$ the linear space of linear, sequentially continuous functionals $T : \mathcal{S} \to \mathbb{C}$ so that $\lim_{n\to\infty} T(\varphi_n) = T(\varphi)$ whenever $\lim_{n\to\infty} \varphi_n = \varphi$ in $\mathcal{S}$. An element in $\mathcal{S}'$ is called a *tempered distribution.*

Problem 2.12. *Show that $\mathcal{D} \subset \mathcal{S}$, that convergence in $\mathcal{D}$ implies convergence in $\mathcal{S}$ and that $\mathcal{S}' \subset \mathcal{D}'$. Show that every $\varphi \in \mathcal{S}$ can be approximated (in $\mathcal{S}$) by a sequence in $\mathcal{D}$, up to errors that vanish asymptotically. Find an example of a distribution $T \in \mathcal{D}'$ which does not admit a continuous extension to $\mathcal{S}$, that is, a distribution which is not tempered.*

In contrast to distributions in $\mathcal{D}'$, a tempered distribution has a well-defined Fourier transform, defined by duality. That is, we define $\widehat{T} \in \mathcal{S}'$ by

$$\widehat{T}(\varphi) := T(\widehat{\varphi}) \;\; \forall\, \varphi \in \mathcal{S}.$$

Problem 2.13. *Prove that $\varphi_n \to \varphi$ in $\mathcal{S}$ implies $\lim_{n\to\infty} \|\varphi - \varphi_n\|_{L^p(\mathbb{R}^d)} = 0$, for every $p \geq 2$, and that $\widehat{\varphi}_n \to \widehat{\varphi}$ in $\mathcal{S}$. Explain why $\widehat{T} \in \mathcal{S}'$ if $T \in \mathcal{S}'$.*

In analogy to classical Fourier properties, we have the following.

Problem 2.14. *Let $T \in \mathcal{S}'$ and $\alpha \in \mathbb{N}_0^d$. Prove that $(\partial^\alpha T) \in \mathcal{S}'$ and that*

$$\widehat{(\partial^\alpha T)} = T(\widehat{2\pi i x^\alpha(\cdot)}) = (2\pi i x^\alpha)\widehat{T}.$$

Let us now conclude the discussion of distributions by stating some further interesting theorems and commenting, through a sequence of problems, on the definition of $\mathcal{S}$ and its dual $\mathcal{S}'$ as locally convex spaces (see [66, 40] and [55, 59] for further details).

Theorem 2.5. *Let $T \in \mathcal{S}'$. Then, there exists some polynomially bounded, continuous function $g \in C(\mathbb{R}^d)$ and some multi-index $\alpha \in \mathbb{N}_0^d$ such that*

$$T(\varphi) = \int_{\mathbb{R}^d} dx\, (-1)^{|\alpha|} g(x)(\partial^\alpha \varphi)(x),$$

that is, every tempered distribution corresponds to some derivative of a mildly growing continuous function.

For the proof of the previous theorem, see [55, Chapter 5]. The following theorem illustrates that the theory of distributions turns out to be quite useful in order to find solutions to partial differential equations.

Theorem 2.6. *Every constant coefficient partial differential operator $L = \sum_{|\alpha|\leq m} c_\alpha \partial^\alpha$ on $\mathbb{R}^d$ admits a fundamental solution, that is, there exists $T \in \mathcal{D}'$ such that $L(T) = \delta$.*

Notice that given a fundamental solution, we have that

$$L(T * \varphi) = (L(T)) * \varphi = \delta * \varphi = \varphi.$$

We thus obtain a smooth solution of the PDE in distributional and hence in the classical sense. The heuristic idea underlying the proof is to find the fundamental solution via

$$T = \int_{\mathbb{R}^d} dp\, \frac{e^{2\pi i p x}}{P(p)},$$

where $P(p) = \sum_{|\alpha|\leq m} c_\alpha (2\pi i p)^\alpha$ denotes the characteristic polynomial of L. Using some tools from complex analysis, one can use the heuristics to construct the fundamental solution $T \in \mathcal{D}'$ rigorously. For the details, see e.g. [66, Chapter 3].

As indicated earlier, the space $\mathcal{S}'$ can be identified with the topological dual space to $\mathcal{S}$ equipped with a suitable topology. We start with the following observation.

Problem 2.15. *Show that $|\cdot|_{\alpha,\beta} : \mathcal{S}(\mathbb{R}^d) \to [0,\infty)$ defines a seminorm, for all $\alpha, \beta \in \mathbb{N}_0^d$. Show that the family of seminorms $(|\cdot|_{\alpha,\beta})_{\alpha,\beta\in\mathbb{N}_0^d}$ separates points.*

Now, let $\tau_{\mathcal{S}}$ denote the weakest topology such that the seminorms $(|\cdot|_{\alpha,\beta})_{\alpha,\beta\in\mathbb{N}_0^d}$ are continuous and let us identify $\mathcal{S} = (\mathcal{S}, \tau_{\mathcal{S}})$ as the topological space with topology $\tau_{\mathcal{S}}$.

Problem 2.16. *Show that an open neighborhood basis around* $0 \in \mathcal{S}$ *is given by the sets*

$$N_{\alpha_1,\beta_2,\dots,\alpha_n,\beta_n,\epsilon} = \Big\{\varphi \in \mathcal{S} : |\varphi|_{\alpha_i,\beta_i} < \epsilon \ \ \forall\, i = 1,\dots,n\Big\} \text{ for } n \in \mathbb{N}, \alpha_i, \beta_i \in \mathbb{N}_0^d \ \forall\, i, \epsilon > 0.$$

Show that $N_{\alpha_1,\beta_2,\dots,\alpha_n,\beta_n,\epsilon}$ *is convex and that* $+ : \mathcal{S}\times\mathcal{S} \to \mathcal{S}$, $\cdot : \mathbb{C}\times\mathcal{S} \to \mathcal{S}$ *are continuous. Finally, prove that* $\varphi_n \to \varphi$ *in* $(\mathcal{S}, \tau_{\mathcal{S}})$ *if and only if* $|\varphi - \varphi_n|_{\alpha,\beta} \to 0$*, for every* $\alpha, \beta \in \mathbb{N}_0^d$*.*

Motivated by the previous problem, one calls $\mathcal{S}$ a *locally convex topological vector space*. Since its topology is induced by a sequence of seminorms, we can also introduce the concept of Cauchy sequences in $\mathcal{S}$: $(\varphi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence if $|\varphi_n - \varphi_m|_{\alpha,\beta} \to 0$ as $n, m \to \infty$, for every $\alpha, \beta \in \mathbb{N}_0^d$.

Problem 2.17. *Show that* $\mathcal{S}$ *is a metrizable space with a metric inducing the same topology and yielding the same Cauchy sequences. Show that* $\mathcal{S}$ *is complete, i.e. every Cauchy sequence has a limit in* $\mathcal{S}$*.*

A complete, metrizable locally convex topological vector space is called a Fréchet space. Now set

$$\mathcal{S}' = \big\{T : \mathcal{S} \to \mathbb{C} : T \text{ is linear and continuous}\big\}$$

and denote by $\tau_{\mathcal{S}'}$ the usual weak-$*$ topology induced by the maps $\iota_\varphi : \mathcal{S}' \to \mathbb{C}$, defined by $\iota_\varphi(T) = T(\varphi)$, for $\varphi \in \mathcal{S}$. The space $(\mathcal{S}', \tau_{\mathcal{S}'})$ is called the space of tempered distributions.

Problem 2.18. *Prove that* $T_n \to T$ *in* $(\mathcal{S}', \tau_{\mathcal{S}'})$ *if and only* $T_n(\varphi) \to T(\varphi)$ *for every* $\varphi \in \mathcal{S}$*. Prove that for every* $T \in \mathcal{S}'$ *there exists* $C > 0$*,* $n \in \mathbb{N}$ *and* $(\alpha_i, \beta_i)_{i=1}^n$ *so that*

$$|T(\varphi)| \le C \sum_{i=1}^n |\varphi|_{\alpha_i,\beta_i} \ \ \forall\, \varphi \in \mathcal{S}.$$

A thorough discussion on $\mathcal{D}(\Omega)$ and its relation to $\mathcal{D}'(\Omega)$ can be found in [59, Chapter 6] (see also [55, Chapter V]). Here, we just record the following basic facts and definitions. Setting for compact $K \subset \Omega$ (with $\Omega \subset \mathbb{R}^d$ open)

$$\mathcal{D}_K = \{\varphi \in C^\infty(\Omega) : \mathrm{supp}(\varphi) \subset K\},$$

we can equip $\mathcal{D}_K$ with the topology τ_K generated by the semi-norms $\|\partial^\alpha(\cdot)\|_\infty$ and it turns out that $\mathcal{D}_K$ becomes a Fréchet space. Now consider sets $V \subset C_c^\infty(\Omega)$ which are convex and balanced ($|\lambda| = 1$ and $\varphi \in V$ implies $\lambda\varphi \in V$) and which are such that $V \cap \mathcal{D}_K \in \tau_K$ for every compact $K \subset \Omega$. Then, we say that a subset

$$U \subset \mathcal{D}(\Omega) = C_c^\infty(\Omega) = \bigcup_{K\subset\Omega: K \text{compact}} \mathcal{D}_K$$

is open in $\mathcal{D}(\Omega)$ if and only if it is of the form $\varphi + V$ for some $\varphi \in C_c^\infty(\Omega)$ and some $V \subset C_c^\infty(\Omega)$ as above. The collection $\tau_{\mathcal{D}}$ of such open sets defines a topology with local base given by the sets V as above and $(\mathcal{D}(\Omega), \tau_{\mathcal{D}})$ defines a complete locally convex topological vector space (which is, however, not metrizable). Moreover, τ_K is equal to the subspace topology of τ restricted to $\mathcal{D}_K$, for every compact $K \subset \Omega$, and convergence in $\mathcal{D}(\Omega)$ is equivalent to the convergence notion introduced earlier. $\mathcal{D}'(\Omega)$ is defined by

$$\mathcal{D}'(\Omega) = \big\{T : \mathcal{D}(\Omega) \to \mathbb{C} : T \text{ is linear and continuous}\big\}$$

and considered a topological space with the weak-$*$ topology induced by the maps $\mathcal{D}'(\Omega) \ni T \mapsto T(\varphi)$, for $\varphi \in \mathcal{D}(\Omega)$. The elements in $\mathcal{D}'(\Omega)$ are called *distributions*.

After this digression on the theory of distributions, let us explain Kato's inequality. We say that a distribution $T \in \mathcal{D}'(\Omega)$ is non-negative if and only if $T(\varphi) \geq 0$ for all $\varphi \in \mathcal{D}$ with $\varphi \geq 0$. Saying that $T_1 \geq T_2$ for $T_1, T_2 \in \mathcal{D}'$ means that $T_1 - T_2 \geq 0$.

Theorem 2.7 (Kato inequality)**.** *Let $u \in L^1_{loc}(\mathbb{R}^d)$ such that its distributional Laplacian Δu is such that $\Delta u \in L^1_{loc}(\mathbb{R}^d)$. Let*

$$(\operatorname{sgn} u)(x) = \begin{cases} 0 & \text{if } u(x) = 0, \\ \overline{u}(x)/|u(x)| & \text{if } u(x) \neq 0 \end{cases}$$

Then $(\operatorname{sgn} u)\Delta u \in L^1_{loc}(\mathbb{R}^d)$ is a distribution. If $\Delta|u|$ denotes the Laplacian of the distribution $|u| \in L^1_{loc}(\mathbb{R}^d)$, we have in distributional sense

$$\Delta|u| \geq \operatorname{Re}\big[(\operatorname{sgn} u)\Delta u\big] \tag{2.9}$$

Proof. The proof consists of two steps. In the first step, we verify (2.9) for smooth functions $u \in C^\infty(\mathbb{R}^d)$. In the second step, we approximate a general $u \in L^1_{\text{loc}}(\mathbb{R}^d)$ by smooth functions to conclude (2.9) for the general case.

Assume first that $u \in C^\infty(\mathbb{R}^d)$. Define for $\varepsilon > 0$ the function $u_\varepsilon \in C^\infty(\mathbb{R}^d)$ pointwise by $u_\varepsilon(x) = \sqrt{|u(x)|^2 + \varepsilon^2}$. If we differentiate $u_\varepsilon^2 = |u|^2 + \varepsilon^2$ at $x \in \mathbb{R}^d$, we find

$$2u_\varepsilon(x)(\nabla u_\varepsilon)(x) = 2\operatorname{Re}\big[\overline{u}(x)(\nabla u)(x)\big]$$

This and $|u| < |u_\varepsilon|$ imply $|(\nabla u_\varepsilon)(x)| \leq |(\nabla u)(x)|$. Moreover, if we take the divergence of the last equation, we find

$$u_\varepsilon(x)(\Delta u_\varepsilon)(x) + |(\nabla u_\varepsilon)(x)|^2 = \operatorname{Re}\big[\overline{u}(x)(\Delta u)(x)\big] + |(\nabla u)(x)|^2$$

so that (first pointwise and therefore) in distributional sense

$$(\Delta u_\varepsilon) \geq \operatorname{Re}\big[(\overline{u}/u_\varepsilon)\Delta u\big] =: \operatorname{Re}\big[\operatorname{sgn}_\varepsilon(u)\Delta u\big]$$

Now, a basic application of the dominated convergence argument for $\varepsilon \to 0$ shows that

$$\Delta|u| \geq \operatorname{Re}\big[\operatorname{sgn}(u)\Delta u\big]$$

in $\mathcal{D}'$, for every $u \in C^\infty(\mathbb{R}^d)$.

Now let $u \in L^1_{\text{loc}}(\mathbb{R}^d)$ as in the assumption and choose an approximate identity of smooth functions $(\varphi_n)_{n\in\mathbb{N}}$ in $C_c^\infty(\mathbb{R}^d)$ so that $\varphi_n = n^d\varphi(n.)$ for some fixed $0 \le \varphi \in C_c^\infty(\mathbb{R}^d)$ with $\int_{\mathbb{R}^d} \varphi(x)\, dx = 1$. Define $u_n = u * \varphi_n \in C^\infty(\mathbb{R}^d)$. Then one verifies that

$$\lim_{n\to\infty} u_n = u, \quad \lim_{n\to\infty} \operatorname{sgn}(u_n)\Delta u_n = \operatorname{sgn}(u)\Delta u$$

in $L^1_{\text{loc}}(\mathbb{R}^d)$ and thus in $\mathcal{D}'$, which concludes (2.9). □

Proposition 2.5. *Let $V \in L^2_{loc}(\mathbb{R}^d)$ be such that $V(x) \ge 0$ for a.e. $x \in \mathbb{R}^d$. Then $-\Delta + V : C_c^\infty(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is essentially self-adjoint.*

Proof. Recall from Theorem 2.2 that the closable symmetric operator $-\Delta+V : C_c^\infty(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ and its closure have the same adjoint $(-\Delta + V)^*$. Since moreover $-\Delta + V \ge 0$ (as an operator) implies that also its closure is non-negative as an operator, the claim follows from Theorem 2.3 and the proof of its corollary if we show

$$\dim(\ker((-\Delta + V + 1)^*)) = 0.$$

Indeed, this implies that $\overline{(-\Delta + V + 1)_{|C_c^\infty}} = (-\Delta + V + 1)^*$. Hence, assume that $(-\Delta + V + 1)^*u = 0$ for $u \in L^2(\mathbb{R}^d)$. Testing against elements from $C_c^\infty(\mathbb{R}^d)$, we get

$$\Delta u = (V + 1)u \in L^1_{\text{loc}}(\mathbb{R}^d)$$

in distributional sense (it is here where we use $V \in L^2_{\text{loc}}(\mathbb{R}^d)$). Hence, Theorem 2.7 yields

$$\Delta|u| \ge \operatorname{Re}\left[\operatorname{sgn}(u)\Delta u\right] = (V + 1)|u| \ge 0.$$

But this implies $u = 0 \in L^2(\mathbb{R}^d)$. In fact, if $|u| \in D(\Delta) = H^2(\mathbb{R}^d)$, this would follow directly from the fact that $\Delta \le 0$ as an operator, together with $u \in L^2(\mathbb{R}^d)$. For a general $u \in L^2(\mathbb{R}^d)$, we define $(|u|_n)_{n\in\mathbb{N}}$ in $H^2(\mathbb{R}^d)$ as $|u|_n = |u| * \varphi_n$ with a sequence $(\varphi_n)_{n\in\mathbb{N}}$ as in the proof of Kato's inequality. Since $\varphi_n \ge 0$ pointwise, we get

$$0 \le \lim_{m\to\infty} \langle \Delta|u|, \varphi_n * (|u|_n\psi_m)\rangle = \langle |u|_n, \Delta|u|_n\rangle \le 0$$

for some $0 \le \psi_m \in C_c^\infty(B_m(0))$, $\psi_m = 1$ in $B_{m/2}(0)$, so that $|u|_n = 0 \in L^2(\mathbb{R}^d)$ for all $n \in \mathbb{N}$. Since $u_n \to u$ in $L^2(\mathbb{R}^d)$, we get $u = 0$. □

Corollary 2.3. *Let $V_{ext} \in L^\infty_{loc}(\mathbb{R}^3)$ be such that $V_{ext}(x) \to \infty$ as $|x| \to \infty$. Moreover, let $v \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with $v \ge 0$ pointwise. Then*

$$H_N^{trap} = \sum_{i=1}^N \big(-\Delta_{x_i} + V_{ext}(x_i)\big) + \sum_{1\le i<j\le N} v(x_i - x_j)$$

is essentially self-adjoint on $C_c^\infty(\mathbb{R}^{3N})$.

The Hamiltonian H_N^{trap} describes N particles trapped in a finite region of $\mathbb{R}^3$ and interacting through the pair potential v. We remark that the assumption $v \ge 0$ in the previous corollary can be dropped. The proof is, however, a bit more involved and eventually we only consider repulsive interactions in the analysis of the Bose gas later on. For a thorough discussion of self-adjointness criteria and its consequences, see [56].

2.4 The Spectral Theorem

In this section, we discuss the Spectral Theorem for self-adjoint operators. We saw already at the beginning of Section 2.3 a short motivation why self-adjoint operators are suitable to describe physically measurable quantities. In the finite dimensional case, one can use them to define spectral measures, associated to the state of the system, that measure the probability of finding the values of an observable in a given interval (or, more generally, in a given Borel subset of $\mathbb{R}$). The spectral theorem shows that this can be done for general self-adjoint operators A: it gives meaning to the operators $\chi_\Omega(A)$, $\Omega \subset \mathcal{B}(\mathbb{R})$, where χ_Ω denotes the characteristic function on Ω. These operators can then be used to measure the probability $\langle \psi, \chi_\Omega(A)\psi\rangle_{\mathcal{H}}$ of finding the value of the observable associated to A in the measurable set Ω if the system is in the state $\psi \in \mathcal{H}$.

The spectral theorem tells us in fact much more. Put in the multiplication operator form, it states that any self-adjoint operator is unitarily equivalent to a multiplication operator as in Proposition 2.1.

Theorem 2.8 (Spectral Theorem, Multiplication Operator Form)**.** *Let $A : D(A) \to \mathcal{H}$ be a self-adjoint operator on the Hilbert space $\mathcal{H}$. Then, there exists a measure space $(\Omega, \mathcal{B}(\Omega), \mu)$, where μ is a finite Borel measure, a unitary map $U : \mathcal{H} \to L^2(\Omega, \mathcal{B}(\Omega), \mu)$ and a real-valued, Ω-a.e. finite μ-measurable function $f : \Omega \to \mathbb{R}$ s.t.*

i) $\psi \in D(A)$ if and only if $f(.)(U\psi)(.) \in L^2(\Omega, \mathcal{B}(\Omega), \mu)$.

ii) If $\varphi \in U(D(A))$, then $(UAU^{-1}(\varphi))(x) = f(x)\varphi(x)$ for μ a.e. $x \in \Omega$.

Clearly, this generalizes the finite dimensional case. In particular, once we have the spectral theorem we can use it to define functions $f(A)$ of A for a suitably large class of functions f. This provides a so called functional calculus. We will see that $\{f(A)\}$ forms a C^*-algebra - an important observation in view of modern axiomatics of quantum mechanics, see e.g. [67]. More important in view of the proof of Theorem 2.8 is that we can turn this picture around - having first a suitable functional calculus, one can deduce Theorem 2.8 by employing the Riesz Representation Theorem 2.25.

The proof of Theorem 2.8 consists of several main steps which are presented below, following [55, Sections VII.1-VII.3; VIII.3].

2.4.1 Spectral Theorem for Bounded Self-Adjoint Operators

In the first step, we develop a functional calculus for bounded, self-adjoint operators. That is, we want to find a reasonable definition for $f(A) \in \mathcal{L}(\mathcal{H})$ when $f \in C(\sigma(A); \mathbb{C})$. Since $\sigma(A) \subset \mathbb{R}$ is compact for any bounded, self-adjoint operator $A \in \mathcal{L}(\mathcal{H})$, we can consider first polynomials of such operators and then use the Stone-Weierstrass Theorem 2.A to extend our map uniquely to continuous functions $f \in C(\sigma(A); \mathbb{C})$. As a preparation we need two lemmas.

Lemma 2.6. *Let $B \in \mathcal{L}(\mathcal{H})$ a bounded operator on $\mathcal{H}$. Let $P \in \mathbb{C}[X]$ be a polynomial in the variable X with complex coefficients such that $P(X) = \sum_{n=0}^{N} a_n X^n$, with $a_n \in \mathbb{C}$*

for $n = 1, \dots, N$. We define $P(A) = \sum_{n=0}^{N} a_n A^n \in \mathcal{L}(\mathcal{H})$. Then

$$\sigma(P(A)) = \{P(\lambda) : \lambda \in \sigma(A)\}$$

Proof. Let $\lambda \in \mathbb{C}$. Then λ is a root of the polynomial $P - P(\lambda)$, which implies that $P(A) - P(\lambda) = (A - \lambda)Q(A)$ for another polynomial $Q : \mathbb{C} \to \mathbb{C}$. Since $Q(A) \in \mathcal{L}(\mathcal{H})$, we conclude that $P(\lambda) \in \rho(P(A))$ implies $\lambda \in \rho(A)$, because in that case

$$\mathbf{1}_{\mathcal{H}} = (A - \lambda)\big(Q(A)(P(A) - P(\lambda))^{-1}\big) = \big(Q(A)(P(A) - P(\lambda))^{-1}\big)(A - \lambda)$$

Thus, $P(\sigma(A)) \subset \sigma(P(A))$.

Next, assume that $\nu \in \sigma(P(A))$ and write $P(A) - \nu = (A - \lambda_1)(A - \lambda_2) \cdots (A - \lambda_N)$ for complex roots $\lambda_n \in \mathbb{C}$, $n = 1, \cdots, N$. Since $\nu \in \sigma(P(A))$, at least one root λ_n must be contained in $\sigma(A)$ (*why*?), denote it by λ. Thus $P(\lambda) - \nu = 0$, i.e. $\nu \in P(\sigma(A))$. □

Lemma 2.7. *Let $A \in \mathcal{L}(\mathcal{H})$ be a bounded normal operator, i.e. $[A, A^*] = 0$, and let $P \in \mathbb{C}[X]$ denote a polynomial in X, as in the previous lemma. Then*

$$\|P(A)\|_{\mathcal{L}(\mathcal{H})} = \sup_{\lambda \in \sigma(A)} |P(\lambda)|.$$

Proof. $P(A)$ is normal if A is normal. Hence

$$\|P(A)\|_{\mathcal{L}(\mathcal{H})} = \lim_{n\to\infty} \|P(A)^n\|_{\mathcal{L}(\mathcal{H})}^{1/n} = r_{P(A)} = \sup_{\lambda \in \sigma(P(A))} |\lambda| = \sup_{\lambda \in \sigma(A)} |P(\lambda)| \qquad (2.10)$$

Notice that we used the identity $\|B^n\|_{\mathcal{L}(\mathcal{H})} = \|B\|_{\mathcal{L}(\mathcal{H})}^n$ for any bounded, normal operator $B \in \mathcal{L}(\mathcal{H})$, which can be proved by induction (*exercise*). The second and third steps are well-known facts from basic functional analysis. □

Note in particular that every bounded self-adjoint operator is normal. Equipped with the two previous lemmas, we deduce the following theorem.

Theorem 2.9 (Continuous Functional Calculus)**.** *Let $A \in \mathcal{L}(\mathcal{H})$ be self-adjoint on $\mathcal{H}$. Then there exists a unique linear map $\Phi : C(\sigma(A); \mathbb{C}) \to \mathcal{L}(\mathcal{H})$ such that*

a) Φ is an algebraic $*$-homomorphism. That is, for all $f, g \in C(\sigma(A); \mathbb{C}), \lambda \in \mathbb{C}$ we have

$$\Phi(fg) = \Phi(f)\Phi(g),\ \Phi(\lambda f) = \lambda\Phi(f),\ \Phi(1) = \mathbf{1}_{\mathcal{H}},\ \Phi(\overline{f}) = \Phi(f)^*$$

b) Φ is bounded with $\|\Phi(f)\|_{\mathcal{L}(\mathcal{H})} = \|f\|_\infty$ for all $f \in C(\sigma(A); \mathbb{C})$.

c) Let $f \in C(\sigma(A); \mathbb{C})$ be defined by $f(x) = x$. Then $\Phi(f) = A$.

In addition, Φ satisfies the following properties.

d) If $A\psi = \lambda\psi$ for some $\psi \in \mathcal{H}, \lambda \in \mathbb{R}$, then $\Phi(f)\psi = f(\lambda)\psi$ for all $f \in C(\sigma(A); \mathbb{C})$.

e) If $f \geq 0$, then $\Phi(f) \geq 0$.

f) $\sigma(\Phi(f)) = \{f(\lambda) : \lambda \in \sigma(A)\} = \operatorname{ran}(f)$ *for all* $f \in C(\sigma(A);\mathbb{C})$.

Remarks:

1) Given $f \in C(\sigma(A);\mathbb{C})$, we write $f(A) = \Phi(f)$.

2) Notice that the image of Φ in $\mathcal{L}(\mathcal{H})$ forms a norm-closed abelian algebra that is closed under adjoints. This is called an abelian C^*-algebra. As indicated earlier, C^*-algebras are the starting point for a modern description of physical systems. For a short introduction to this viewpoint, see for instance [67, Chapters 1 and 2].

Proof. We apply Lemmas 2.6, 2.7 and the Stone-Weierstrass Theorem 2.24. We define

$$\Phi(P) = P(A)$$

for any polynomial $P \in \mathbb{C}[X]$. The set of polynomials, viewed as functions from $\sigma(A) \subset \mathbb{R}$ to $\mathbb{C}$, is dense in $C(\sigma(A);\mathbb{C})$ by Theorem 2.24 (*why do the polynomials separate points?*), and by Lemma 2.7 Φ can be extended to a linear isometry from $C(\sigma(A);\mathbb{C})$ to $\mathcal{L}(\mathcal{H})$. Using that $A = A^*$, properties $a), b), c), d)$ are true for polynomials and carry over to $C(\sigma(A);\mathbb{C})$ by density. Also, $a), b), c)$ and the linearity of Φ determine Φ on the set of polynomials, because

$$\Phi\Big(\sum_j \alpha_j X^j\Big) = \sum_j \alpha_j A^j$$

By a density argument, this shows that $a), b), c)$ and linearity characterize Φ uniquely. Notice indeed that it is enough to assume $\|\Phi(f)\|_{\mathcal{L}(\mathcal{H})} \leq \|f\|_\infty$ for all $f \in C(\sigma(A);\mathbb{C})$ in order to prove uniqueness of the continuous functional calculus.

To prove $e)$, we write $f = (\sqrt{f})^2$ and use $a)$ which implies

$$\Phi(f) = \Phi(\sqrt{f})^2 = \Phi(\sqrt{f})^*\Phi(\sqrt{f}) \geq 0.$$

To prove $f)$, assume first $z \notin \operatorname{ran}(f)$. Then $(f-z)^{-1} \in C(\sigma(A);\mathbb{C})$ exists with

$$\|(f-z)^{-1}\|_\infty \leq \frac{1}{\operatorname{dist}(f(\sigma(A)), z)} < \infty$$

and we have

$$\mathbf{1}_{\mathcal{H}} = \Phi((f-z)(f-z)^{-1}) = (\Phi(f)-z)\Phi((f-z)^{-1}) = \Phi((f-z)^{-1})(\Phi(f)-z),$$

so that $z \in \rho(\Phi(f))$. This shows that $\sigma(\Phi(f)) \subset f(\sigma(A))$.

On the other hand, assume that $z \in \sigma(A)$, then for any polynomial $P \in \mathbb{C}[X]$, we have $P(z) \in \sigma(P(A))$. That is, $P(A) - P(z)$ does not have a bounded inverse. Writing

$$\Phi(f) - f(z) = \lim_{n\to\infty} (P_n(A) - P_n(z)) \in \mathcal{L}(\mathcal{H})$$

for a suitable sequence of polynomials $(P_n)_{n\in\mathbb{N}}$, we conclude that $f(z) \in \sigma(\Phi(f))$, because the set of operators with bounded inverse is open[4] in $\mathcal{L}(\mathcal{H})$, so $f(\sigma(A)) \subset \sigma(\Phi(f))$. □

[4]Indeed, if $A \in \mathcal{L}(\mathcal{H})$ has inverse $A^{-1} \in \mathcal{L}(\mathcal{H})$, the inverse of $B = A(1 + A^{-1}(B-A))$ exists if $\|B-A\|_{\mathcal{L}(\mathcal{H})} < \|A^{-1}\|^{-1}_{\mathcal{L}(\mathcal{H})}$ by a standard Neumann expansion.

With the continuous functional calculus at hand, we can prove the analogue of Theorem 2.8 for bounded self-adjoint operators. First of all, we need to relate A to a suitable measure space. The crucial observation is that, given any $\psi \in \mathcal{H}$, the map

$$C(\sigma(A);\mathbb{C}) \ni f \mapsto \langle \psi, f(A)\psi \rangle_{\mathcal{H}} \in \mathbb{C}$$

is a positive, linear functional. By the Riesz Representation Theorem 2.25, there exists a unique, positive Borel measure $\mu_\psi^A : \mathcal{B}(\mathbb{R}) \to [0,\infty)$ s.t.

$$\langle \psi, f(A)\psi \rangle_{\mathcal{H}} = \int_{\sigma(A)} f(x)\, d\mu_\psi^A(x), \qquad \forall f \in C(\sigma(A);\mathbb{C}). \tag{2.11}$$

We call μ_ψ^A the spectral measure of A associated with the vector $\psi \in \mathcal{H}$. The connection to L^2-spaces comes from noticing that 2.11 implies that for all $f \in C(\sigma(A);\mathbb{C})$ we have

$$\|f(A)\psi\|_{\mathcal{H}} = \langle \psi, \overline{f}(A)f(A)\psi \rangle_{\mathcal{H}} = \langle \psi, |f(A)|^2\psi \rangle_{\mathcal{H}} = \int_{\sigma(A)} |f(x)|^2\, d\mu_\psi^A(x) \tag{2.12}$$

If we knew that $\mathcal{H} = \overline{\{f(A)\psi : f \in C(\sigma(A);\mathbb{C})\}}$ $(= \overline{\operatorname{span}\{f(A)\psi : f \in C(\sigma(A);\mathbb{C})\}}\,)$ for some fixed vector[5] $\psi \in \mathcal{H}$, equation (2.12) would immediately imply Theorem 2.8 for bounded self-adjoint operators, with the self-adjoint operator A being unitarily equivalent to multiplication by the function $\sigma(A) \ni x \mapsto f_A(x) = x$. Notice in particular that $C(\sigma(A);\mathbb{C})$ is dense in $L^2(\sigma(A), \mathcal{B}(\sigma(A)), \mu_\psi^A)$, whose proof uses that the measure μ_ψ^A is regular (indeed, one may approximate first a characteristic function of some Borel set B by a characterstic function of some open set $O \supset B$ and some compact set $K \subset B$, by regularity of μ_ψ^A. Then we can find a continuous function which is equal to one on K and shrinks to zero when we approach the complement of B). However, in general

$$\overline{\{f(A)\psi : f \in C(\sigma(A);\mathbb{C})\}} \subsetneq \mathcal{H}.$$

Lemma 2.8. *Let $A \in \mathcal{L}(\mathcal{H})$ be self-adjoint on the separable Hilbert space $\mathcal{H}$. Then, there exists a direct sum decomposition $\mathcal{H} = \bigoplus_n^N \mathcal{H}_n$ with $N \in \mathbb{N}$ or $N = \infty$ such that for each $n \in \mathbb{N}$, there exists some $\varphi_n \in \mathcal{H}$ s.t. $\mathcal{H}_n = \overline{\{f(A)\varphi_n : f \in C(\sigma(A);\mathbb{C})\}}$.*

Proof. We proceed inductively. Choose an ONB $\{\varphi_i : i \in \mathbb{N}\} \subset \mathcal{H}$ of $\mathcal{H}$ and define

$$\mathcal{H}_1 = \overline{\{f(A)\psi_1 : f \in C(\sigma(A);\mathbb{C})\}}$$

for $\psi_1 = \varphi_1$. We decompose $\mathcal{H}$ into the direct sum $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_1^\perp$ and denote by $P_1^\perp \in \mathcal{L}(\mathcal{H})$ the orthogonal projection onto $\mathcal{H}_1^\perp$. If $\mathcal{H} = \mathcal{H}_1$, we are done. If not, pick the smallest $i_1 \in \mathbb{N} \setminus \{1\}$ such that $\varphi_{i_1} \notin \mathcal{H}_1$. Now, we repeat the first step with $\psi_2 = P_1^\perp \varphi_{i_2} / \|P_1^\perp \varphi_{i_2}\|_{\mathcal{H}}$. Notice that $\psi_2 \in \mathcal{H}_1^\perp$ and that $\mathcal{H}_1^\perp$ is invariant under the action of $g(A)$, for every $g \in C(\sigma(A);\mathbb{C})$. Indeed, if $\psi \in \mathcal{H}_1^\perp$, then for every $g \in C(\sigma(A);\mathbb{C})$ and $f \in C(\sigma(A);\mathbb{C})$, we have that

$$\langle f(A)\varphi_1, g(A)\psi \rangle = \langle (f\overline{g})(A)\varphi_1, \psi \rangle = 0.$$

[5] A vector $\psi \in \mathcal{H}$ with the property that $\mathcal{H} = \overline{\operatorname{span}\{A^n\psi : n \in \mathbb{N}_0\}}$ is called cyclic for A.

Picking $\psi_2 = P_1^\perp \varphi_{i_2}/\|P_1^\perp \varphi_{i_2}\|_{\mathcal{H}}$ as above, we thus obtain a direct sum decomposition

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \big(\mathcal{H}_1 \oplus \mathcal{H}_2\big)^\perp,\ \mathcal{H}_j = \overline{\{f(A)\psi_j : f \in C(\sigma(A);\mathbb{C})\}}\ (j = 1, 2),$$

with $\{\varphi_1, \dots, \varphi_{i_1}\} \subset \mathcal{H}_1 \oplus \mathcal{H}_2$.

Iterating this procedure, we obtain a possibly finite sequence $(\psi_n)_{n\in\mathbb{N}}$ of normalized vectors in $\mathcal{H}$ with associated orthogonal subspaces $(\mathcal{H}_n)_{n\in\mathbb{N}}$ so that ψ_n is cyclic for $\mathcal{H}_N$ and which are A-invariant. By construction, we have that

$$\psi \in \Big(\bigoplus_n^N \mathcal{H}_n\Big)^\perp \implies \psi \in \big\{\varphi_i : i \in \mathbb{N}\big\}^\perp = \{0\},$$

so that $\mathcal{H} = \bigoplus_n^N \mathcal{H}_n$. □

Theorem 2.10. *Let $A \in \mathcal{L}(\mathcal{H})$ be self-adjoint on the Hilbert space $\mathcal{H}$. Then, there exist finite, positive Borel measures $(\mu_n^A)_{1\leq n\leq N}$ where $N \in \mathbb{N}$ or $N = \infty$, and a unitary map $U : \mathcal{H} \to \bigoplus_{n=1}^N L^2\big(\sigma(A), \mathcal{B}(\sigma(A)), \mu_n^A\big)$ such that*

$$(UAU^{-1}g)_n(x) = xg_n(x), \quad \textit{for } \mu \textit{ a.e. } x \in \sigma(A), \forall\, 1 \leq n \leq N \tag{2.13}$$

for all $g = (g_n)_{1\leq n\leq N} \in \bigoplus_{n=1}^N L^2\big(\sigma(A), \mathcal{B}(\sigma(A)), \mu_n^A\big)$.

Proof. We decompose $\mathcal{H} = \bigoplus_n^N \mathcal{H}_n$ with $\mathcal{H}_n = \overline{\{f(A)\varphi_n : f \in C(\sigma(A);\mathbb{C})\}}$ as in Lemma 2.8. The map U is defined componentwise on each $\mathcal{H}_n$. For $\psi_n = f(A)\varphi_n \in \mathcal{H}_n$ with $f \in C(\sigma(A);\mathbb{C})$, we define $U\psi_n = f \in C(\sigma(A);\mathbb{C})$. By (2.12), U extends to a linear isometry from $\mathcal{H}_N$ to $L^2\big(\sigma(A), \mathcal{B}(\sigma(A)), \mu_n^A\big)$ where μ_n^A is the spectral measure of A w.r.t. $\varphi_n \in \mathcal{H}_n$. Notice here that we use the fact that $C(\sigma(A);\mathbb{C})$ is dense in $L^2\big(\sigma(A), \mathcal{B}(\sigma(A)), \mu_n^A\big)$. Since $\sigma(A) \ni x \mapsto x$ continuous, we conclude (2.13). □

The following corollary shows that every self-adjoint, bounded operator is unitarily equivalent to a multiplication operator of the same form as in Proposition 2.1.

Corollary 2.4. *Let $A \in \mathcal{L}(\mathcal{H})$ be self-adjoint on the Hilbert space $\mathcal{H}$. Then, there exists a finite measure space $(M, \mathcal{B}(M), \mu)$ with μ a Borel measure, a unitary map $U : \mathcal{H} \to L^2(M, \mathcal{B}(M), \mu)$ and a bounded, measurable function $f : M \to \mathbb{R}$ such that for all $\psi \in L^2(M, \mathcal{B}(M), \mu)$*

$$(UAU^{-1}\psi)(x) = f(x)\psi(x), \quad \textit{for } \mu \textit{ a.e. } x \in M \tag{2.14}$$

Proof. With the same notation as in the proof of Theorem 2.10, we choose the cyclic vectors $\varphi_i \in \mathcal{H}_i$ s.t. $\|\varphi_i\|_{\mathcal{H}} = 2^{-i}$. We then define M as the disjoint union

$$M = \coprod_{i=1}^N \sigma(A) = \big\{(i, x) : i \in \{1, \dots, N\}, x \in \sigma(A)\big\}$$

with its Borel σ-algebra (the smallest σ-algebra generated by the open sets in M). Recall that M is equipped with the finest topology such that the injections $\Phi_i : \sigma(A) \to M$, for $i = 1, \ldots, N$ (the index referring to the i-th copy of the spectrum $\sigma(A)$), defined by

$$\Phi_i(x) = (i, x) \in M,$$

are continuous. More precisely, a set $U = \coprod_{i=1}^N U_i \subset M$ is open if and only if $\Phi_i^{-1}(U) = U_i \subset \sigma(A)$ is open, for all $i = 1, \ldots, N$. Given M, we then define μ through

$$\mu\Big(\coprod_{i=1}^N O_i\Big) = \sum_{i=1}^N \mu_i^A(O_i),$$

so that $\mu(M) = \sum_{i=1}^N \mu_i^A(\sigma(A)) = \sum_{i=1}^N 2^{-2i} < \infty$. The previous identity means that

$$\int_M d\mu\, \chi_{\coprod_{i=1}^N O_i} = \sum_{i=1}^N \int_{\sigma(A)} d\mu_i^A\, \chi_{O_i}$$

for measurable sets $O_i \in \mathcal{B}(\sigma(A))$, $i = 1, \ldots, N$. Hence, writing $\psi \in L^2(M, \mathcal{B}(M), \mu)$ as

$$\psi = \sum_{i=1}^N \psi_i \chi_{\emptyset \coprod \cdots \coprod \sigma(A) \coprod \cdots \coprod \emptyset}$$

for $\psi_i = \psi_{|(i,\cdot)} : \sigma(A) \to \mathbb{C}$ denoting the restriction of ψ to the i-th copy of $\sigma(A)$, and using the orthogonality of the different summands in $L^2(M, \mathcal{B}(M), \mu)$, we conclude that

$$\int_M \mu(d\omega)\, |\psi(\omega)|^2 = \sum_{i=1}^N \int_{\sigma(A)} \mu_i^A(dx) |\psi_i(x)|^2.$$

In other words, the map

$$L^2(M, \mathcal{B}(M), \mu) \ni \psi \mapsto (\psi_1, \ldots, \psi_N) \in \bigoplus_{i=1}^N L^2\big(\sigma(A), \mathcal{B}(\sigma(A)), \mu_i^A\big),$$

is a unitary map and it is straightforward to check that A acts in $L^2(M, \mathcal{B}(M), \mu)$ as $(UAU^{-1}\psi)(i, x) = f(i, x)\psi(i, x) = x\psi_i(x)$ for each $i = 1, \ldots, N$ and $x \in \sigma(A)$. □

2.4.2 Spectral Theorem for Bounded Normal Operators

In this section, we explain the main ideas on how to extend the spectral theorem from bounded, self-adjoint operators to bounded, normal operators. This extension enables us to prove the spectral theorem for unbounded operators. The strategy one should have in mind is that, given an unbounded self-adjoint operator, its resolvent is a bounded, normal operator. If we knew that such operators are equivalent to multiplication operators, we would deduce that also the original operator is unitarily equivalent to a multiplication operator. An important question is then: why can we expect the spectral theorem for normal, bounded operators to hold? The key is that a normal operator is the sum of two commuting self-adjoint operators and we can develop a functional calculus for such a pair of operators. Some details of the arguments are skipped and we refer the interested reader to [51, Chapter 5] and [55, Chapter VII, Problems 4,5].

Before we explain the spectral theorem for bounded, normal operators, let's observe that we can extend the continuous functional calculus from Theorem 2.9 to the set of bounded, Borel measurable functions on $\mathbb{R}$, denoted by $\mathcal{M}(\mathbb{R})$. Indeed, with the notation from Corollary 2.4, we may define $f(A) \in \mathcal{L}(\mathcal{H})$ for a given $f \in \mathcal{M}(\mathbb{R})$ via[6]

$$(Uf(A)U^{-1}\psi)(x) = (f \circ g)(x)\psi(x), \quad \text{for } \mu \text{ a.e. } x \in M,$$

if A corresponds to multiplication by g in $L^2(M, d\mu)$. With this definition, we derive similarly to Theorem 2.9 the following measurable functional calculus.

Theorem 2.11 (Measurable Functional Calculus). *Let $A \in \mathcal{L}(\mathcal{H})$ be self-adjoint on $\mathcal{H}$. Then there exists a unique linear map $\widehat{\Phi} : \mathcal{M}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ such that*

a) $\widehat{\Phi}$ is an algebraic $*$-homomorphism.

b) $\widehat{\Phi}$ is bounded with $\|\widehat{\Phi}(f)\|_{\mathcal{L}(\mathcal{H})} \leq \|f\|_\infty$ for all $f \in \mathcal{M}(\mathbb{R})$.

c) Let $(f_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{M}(\mathbb{R})$ s.t. $|f_n(x)| \leq |x|$ for all $n \in \mathbb{N}$, $x \in \mathbb{R}$ and $\lim_{n\to\infty} f_n(x) = x$ for all $x \in \mathbb{R}$. Then $(\widehat{\Phi}(f_n))_{n\in\mathbb{N}}$ converges strongly *to A.*

d) Let $f \in \mathcal{M}(\mathbb{R})$ and let $(f_n)_{n\in\mathbb{N}}$ be a bounded sequence in $\mathcal{M}(\mathbb{R})$. Assume that f_n converges to f pointwise in $\mathbb{R}$, then $\widehat{\Phi}(f_n)$ converges strongly *to $\widehat{\Phi}(f)$.*

In addition, $\widehat{\Phi}$ satisfies the following properties.

e) If $A\psi = \lambda\psi$ for some $\psi \in \mathcal{H}, \lambda \in \mathbb{R}$, then $\widehat{\Phi}(f)\psi = f(\lambda)\psi$ for all $f \in \mathcal{M}(\mathbb{R})$.

f) If $f \geq 0$, then $\widehat{\Phi}(f) \geq 0$.

g) If $[A, B] = 0$ for some $B \in \mathcal{L}(\mathcal{H})$, then $[\widehat{\Phi}(f), B] = 0$ for all $f \in \mathcal{M}(\mathbb{R})$.

Proof. By Corollary 2.4, we can assume w.l.o.g. that A corresponds to multiplication by some measurable function $g : M \to \mathbb{R}$ on $L^2(M, \mathcal{B}(M), \mu) =: L^2(d\mu)$. Then we define $\widehat{\Phi}(f)\,(= f(A))$ through multiplication by $f \circ g \in \mathcal{M}(\mathbb{R})$, for $f \in \mathcal{M}(\mathbb{R})$. The properties $a)$ to $d)$ are straightforward to verify (notice that the inequality in $b)$ may be strict - *exercise*). For example, for part $d)$, the dominated convergence theorem implies

$$\|(f(A) - f_n(A))\psi\|_2^2 = \int_M d\mu(x)\, |f \circ g(x) - f_n \circ g(x)|^2 |\psi(x)|^2 \to 0$$

[6] Notice that for bounded operators $A \in \mathcal{L}(\mathcal{H})$, our definition makes sense for a larger class of functions, including those which need not be bounded in $\mathbb{R}$. In view of the functional calculus for general (possibly unbounded) self-adjoint operators, we formulate the functional calculus nevertheless in terms of $\mathcal{M}(\mathbb{R})$.

as $n \to \infty$, for every $\psi \in L^2(d\mu)$, if $\lim_{n\to\infty} f_n(x) = f(x)$ for all $x \in M$ for a bounded sequence $(f_n)_{n\in\mathbb{N}}$ in $\mathcal{M}(\mathbb{R})$.

For part *e*), notice that if $A\psi = \lambda\psi$, then ψ is supported in $g^{-1}(\{\lambda\}) \subset M$ and thus $\big(f(A)\psi\big)(x) = f(\lambda)\psi(x)$ for *a.e.* $x \in M$. Similarly, we argue for part *f*).

To prove *g*), we first argue that $[\chi_{(a,b)}(A), B] = 0$ for all $-\infty \le a \le b \le \infty$. Here, we use that, by the Stone-Weierstrass Theorem 2.24, the closed *-subalgebra of

$$C_\infty(\mathbb{R}) = \big\{ f \in C(\mathbb{R};\mathbb{C}) : \lim_{|x|\to\infty} f(x) = 0 \big\} \ \big(\subset \mathcal{M}(\mathbb{R}) \big)$$

generated by $x \mapsto (x-i)^{-1}, x \mapsto (x+i)^{-1}$ is dense in $C_\infty(\mathbb{R})$ (w.r.t. $\|\cdot\|_\infty$). In fact, this subalgebra separates points (*why?*) and is closed under complex conjugation in

$$\big\{ f \in C(X) : f(\pm\infty) = 0 \big\},$$

where $X = \mathbb{R} \cup \{\pm\infty\}$ denotes the extended real numbers (as a compactification of $\mathbb{R}$). Observe here that $C_\infty(\mathbb{R})$ is isometrically isomorphic to $C(X)$.

Since $[A, B] = 0 = [\mathbf{1}_{\mathcal{H}}, B]$, it follows that

$$(A+i)[(A+i)^{-1}, B] = 0 = [(A+i)^{-1}, B](A+i),$$

which implies that $[(A+i)^{-1}, B] = 0$, because $(A+i) : \mathcal{H} \to \mathcal{H}$ is invertible. Similarly, $[(A-i)^{-1}, B] = 0$ so that by part *d*), we conclude $[f(A), B] = 0$ for every $f \in C_\infty(\mathbb{R})$. Then, another application of *d*) shows that $[\chi_{(a,b)}(A), B] = 0$ for all $-\infty \le a \le b \le \infty$.

To conclude *g*), consider now the set $\mathcal{A} = \big\{ S \subset \mathbb{R} : [\chi_S(A), B] = 0 \big\}$. Our previous arguments imply that $\mathcal{A}$ contains every open set (*why?*) and we also observe that $\mathcal{A}$ is a σ-algebra. In fact, using that

$$\chi_{S^c}(A) = \chi_{\mathbb{R}}(A) - \chi_S(A) = 1 - \chi_S(A), \qquad \chi_{S_1\cap S_2}(A) = \chi_{S_1}(A)\chi_{S_2}(A),$$
$$\chi_{\cup_{j=1}^\infty S_j}(A) = \sum_{j=1}^\infty \chi_{S_j}(A) \ \ (\text{if } S_i \cap S_j = \delta_{ij}),$$

we conclude that $\mathcal{A}$ is a Dynkin system stable under intersections. Since it contains the open sets, $\mathcal{B}(\mathbb{R}) \subset \mathcal{A}$. Finally, every $f \in \mathcal{M}(\mathbb{R})$ can be approximated pointwise (everywhere) by a sequence of simple functions s.t. $[f(A), B] = 0$ for all $f \in \mathcal{M}(\mathbb{R})$.

Let's switch to the uniqueness of the functional calculus. Suppose that $\widehat{\Phi}$ and $\widehat{\Psi}$ both satisfy properties *a*) to *g*). Using parts *a*), *c*) and *d*), we first deduce that

$$\mathbf{1}_{\mathcal{H}} = \widehat{\Phi}\big(x \mapsto (x \pm i)^{-1}\big)(A \pm i) = (A+i)\widehat{\Phi}\big(x \mapsto (x \pm i)^{-1}\big),$$

so that $\widehat{\Phi}\big(x \mapsto (x \pm i)^{-1}\big) = (A \pm i)^{-1} = \widehat{\Psi}\big(x \mapsto (x \pm i)^{-1}\big)$ (arguing analogously for $\widehat{\Psi}$). As in the proof of *g*), this implies that $\widehat{\Phi}(f) = \widehat{\Psi}(f)$ for all $f \in C_\infty(\mathbb{R})$. Applying *d*) once more, we deduce that $\widehat{\Phi}(\chi_S) = \widehat{\Psi}(\chi_S)$ for all $S \in \mathcal{B}(\mathbb{R})$ and then $\widehat{\Phi} = \widehat{\Psi}$ in $\mathcal{M}(\mathbb{R})$. □

Now, let's explain how to use the measurable functional calculus to prove the spectral theorem for bounded, normal operators. Let $A \in \mathcal{L}(\mathcal{H})$ be normal, i.e. $[A, A^*] = 0$.

Then we can define two bounded, self-adjoint operators $B = \frac{1}{2}(A + A^*) \in \mathcal{L}(\mathcal{H})$ and $C = \frac{1}{2i}(A - A^*) \in \mathcal{L}(\mathcal{H})$ that satisfy

$$A = B + i\,C, \quad B = B^*, \quad C = C^*, \quad [B, C] = 0$$

We have already a functional calculus for B and C, separately, but what we need now is a joint functional calculus for B and C. To this end, we proceed in the following steps:

1) Denote by Y the product space $Y = Y_1 \times Y_2 = \sigma(B) \times \sigma(C)$. Let $f \in \mathcal{M}(Y)$ be a finite linear combination of characteristic functions of the form $\chi = \chi_{\Omega_1} \otimes \chi_{\Omega_2} \in \mathcal{M}(Y)$ for measurable subsets $\Omega_i \in \mathcal{B}(Y_i), i = 1, 2$. We define $\chi(B, C) = \chi_{\Omega_1}(B)\chi_{\Omega_2}(C) \in \mathcal{L}(\mathcal{H})$ and then $f(B, C) \in \mathcal{L}(\mathcal{H})$ by linearity. For such $f \in \mathcal{M}(Y)$, we have

$$\|f(B, C)\|_{\mathcal{L}(\mathcal{H})} \le \sup_{y \in Y} |f(y)|. \tag{2.15}$$

If $f = \chi_{\Omega_1} \otimes \chi_{\Omega_2} \subset \mathcal{M}(Y)$, this follows in fact from Theorem 2.11 *b*), $\chi_\emptyset(B) = \chi_\emptyset(C) = 0$ and $\sup_{y \in Y} |\chi_{\Omega_1} \otimes \chi_{\Omega_2}| = \sup_{y_1 \in Y_1} |\chi_{\Omega_1}(y_1)| \sup_{y_2 \in Y_2} |\chi_{\Omega_2}(y_2)|$. If

$$(\Omega_1^{(i)} \times \Omega_2^{(i)}) \cap (\Omega_1^{(j)} \times \Omega_2^{(j)}) = \emptyset \;\; \big(= (\Omega_1^{(i)} \cap \Omega_1^{(j)}) \times (\Omega_2^{(i)} \cap \Omega_2^{(j)})\big),$$

we therefore have that $\chi_{\Omega_1^{(i)} \cap \Omega_1^{(j)}} \otimes \chi_{\Omega_2^{(i)} \cap \Omega_2^{(j)}}(B, C) = 0$.

Now, if f is a linear combination of characteristic functions, we may write

$$f = \sum_{i=1}^{n} \lambda_i \chi_{\Omega_1^{(i)}} \otimes \chi_{\Omega_2^{(i)}}, \qquad (\Omega_1^{(i)} \times \Omega_2^{(i)}) \cap (\Omega_1^{(j)} \times \Omega_2^{(j)}) = \emptyset \;\text{ for } i \ne j.$$

By Theorem 2.11 *g*), we have $[\chi_{\Omega_1}(B), \chi_{\Omega_2}(C)] = 0$. Therefore, we find that

$$\begin{aligned}
&\langle \chi_{\Omega_1^{(i)}} \otimes \chi_{\Omega_2^{(i)}}(B, C)\psi, \chi_{\Omega_1^{(j)}} \otimes \chi_{\Omega_2^{(j)}}(B, C)\psi \rangle_{\mathcal{H}} \\
&\quad = \big\langle \big(\chi_{\Omega_1^{(i)}} \chi_{\Omega_1^{(j)}}\big)(B)\psi, \big(\chi_{\Omega_2^{(i)}} \chi_{\Omega_2^{(j)}}\big)(C)\psi \big\rangle_{\mathcal{H}} \\
&\quad = \langle \chi_{\Omega_1^{(i)} \cap \Omega_1^{(j)}}(B)\psi, \chi_{\Omega_2^{(i)} \cap \Omega_2^{(j)}}(C)\psi \rangle_{\mathcal{H}} \\
&\quad = \langle \psi, \chi_{\Omega_1^{(i)} \cap \Omega_1^{(j)}} \otimes \chi_{\Omega_2^{(i)} \cap \Omega_2^{(j)}}(B, C)\psi \rangle_{\mathcal{H}} = 0
\end{aligned}$$

for every $\psi \in \mathcal{H}$ and $i \ne j$ so that

$$\|f(B, C)\psi\|_{\mathcal{H}}^2 \le \sum_{i=1}^{n} |\lambda_i|^2 \langle \psi, \chi_{\Omega_1^{(i)}} \otimes \chi_{\Omega_2^{(i)}}(B, C)\psi \rangle_{\mathcal{H}} \le \sup_{i=1,\dots,N} |\lambda_i|^2 \|\psi\|_{\mathcal{H}}^2.$$

2) Given $f \in C(Y; \mathbb{C})$, we approximate it uniformly in Y by a sequence of simple functions as in Step 1). Then we construct a continuous functional calculus as in Theorem 2.9. More precisely, we define a map $\Sigma : C(Y; \mathbb{C}) \to \mathcal{L}(\mathcal{H})$ satisfying

   a) Σ is an algebraic *-homomorphism.

b) Σ is bounded with $\|\Sigma(f)\|_{\mathcal{L}(\mathcal{H})} \leq \|f\|_\infty$ for all $f \in C(Y;\mathbb{C})$.

c) Let $f \in C(Y;\mathbb{C})$ be defined by $f(y_1, y_2) = y_1 + iy_2$. Then $\Sigma(f) = B + iC = A$.

d) If $f \in C(Y;\mathbb{C})$ satisfies $f \geq 0$, then $\Sigma(f) \geq 0$.

We write $\Sigma(f) = f(B,C)$. Note that restricting Σ to $C(\sigma(B);\mathbb{C}) \hookrightarrow C(Y;\mathbb{C})$ or to $C(\sigma(C);\mathbb{C}) \hookrightarrow C(Y;\mathbb{C})$ yields a continuous functional calculus for B and, respectively, C. Therefore, the identity $\Sigma(f) = B + iC = A$ in c) follows by uniqueness of the continuous functional calculus (for B and, respectively, C) and by linearity.

3) We observe that for $f, g \in \mathcal{M}(Y)$, $\psi \in \mathcal{H}$ and $A = B + iC$, we find some finite, positive Borel measure μ_ψ such that

$$\langle f(B,C)\psi, Ag(B,C)\psi\rangle_{\mathcal{H}} = \int_Y \mu_\psi(dy_1 dy_2)\overline{f}(y_1, y_2)(y_1 + iy_2)g(y_1, y_2).$$

Thus, A is represented on $L^2(d\mu_\psi)$ as the multiplication operator that multiplies with $(y_1, y_2) \mapsto y_1 + iy_2$. We then proceed as in Section 2.4.1 and prove the following.

Theorem 2.12. *Let $A \in \mathcal{L}(\mathcal{H})$ be normal on the Hilbert space $\mathcal{H}$. Then, there exists a finite measure space $(M, \mathcal{B}(M), \mu)$ with μ a Borel measure, a unitary map $U : \mathcal{H} \to L^2(M, \mathcal{B}(M), \mu)$ and a bounded, measurable function $f : M \to \mathbb{C}$ such that for all $\psi \in L^2(M, \mathcal{B}(M), \mu)$*

$$(UAU^{-1}\psi)(x) = f(x)\psi(x), \quad \textit{for } \mu \textit{ a.e. } x \in M \tag{2.16}$$

Moreover, A is self-adjoint if and only if the function $f : M \to \mathbb{C}$ is real-valued.

Problem 2.19. *Give a detailed proof of Theorem 2.12.*

2.4.3 Spectral Theorem for Unbounded Self-Adjoint Operators

We are now ready to prove the spectral theorem in the general, unbounded case.

Proof of Theorem 2.8. Let $A : D(A) \to \mathcal{H}$ be self-adjoint. The resolvents $(A - i)^{-1}$ and $(A + i)^{-1} \in \mathcal{L}(\mathcal{H})$ commute and they are normal, because $\big((A - i)^{-1}\big)^* = (A + i)^{-1}$. Moreover, we have that $D(A) = \operatorname{ran}(A - i)^{-1} = \operatorname{ran}(A + i)^{-1}$. By Theorem 2.12, there exists a finite measure space $(\Omega, \mathcal{B}(\Omega), \mu)$ with μ a Borel measure, a unitary map $U : \mathcal{H} \to L^2(\Omega, \mathcal{B}(\Omega), \mu)$ and a function $g : \Omega \to \mathbb{C}$ such that for all $\varphi \in L^2(\Omega, \mathcal{B}(\Omega), \mu)$

$$(U(A + i)^{-1}U^{-1}\varphi)(x) = g(x)\varphi(x), \quad \text{for } \mu \textit{ a.e. } x \in \Omega,\ \forall \varphi \in L^2(\Omega, \mathcal{B}(\Omega), \mu) \tag{2.17}$$

Since $\ker(A + i)^{-1} = \{0\}$, we must have $g(x) \neq 0$ for *a.e.* $x \in \Omega$, because otherwise $0 \neq U^{-1}\chi_{g^{-1}(\{0\})} \in \ker(A + i)^{-1}$. Therefore, the measurable function f defined by

$$f(x) = g(x)^{-1} - i \quad \big(\Leftrightarrow g(x) = (f(x) + i)^{-1}\big)$$

is finite for μ *a.e.* $x \in \Omega$.

Now, let $\psi \in D(A)$. Then $\psi = (A+i)^{-1}\varphi$ for some $\varphi \in \mathcal{H}$. Hence, we have that

$$U(\psi) = \big(U(A+i)^{-1}U^{-1}\big)U(\varphi) = g\,U(\varphi) \in L^2(\Omega, \mathcal{B}(\Omega), \mu)$$

and thus

$$fU\psi = (fg)U(\varphi) = (1-ig)U(\varphi) \in L^2(\Omega, \mathcal{B}(\Omega), \mu).$$

Conversely, if $f\,U(\psi) = (g^{-1}-i)U(\psi) \in L^2(\Omega, \mathcal{B}(\Omega), \mu)$, then $g^{-1}U(\psi) \in L^2(\Omega, \mathcal{B}(\Omega), \mu)$, because $U(\psi) \in L^2(\Omega, \mathcal{B}(\Omega), \mu)$. Writing

$$g^{-1}U(\psi) = U(U^{-1}g^{-1}U(\psi)) = U(\varphi) \text{ for } \varphi = U^{-1}g^{-1}U(\psi) \in \mathcal{H},$$

this implies $U(\psi) = g\,U(\varphi) = U(A+i)^{-1}\varphi$ so that $\psi = (A+i)^{-1}\varphi \in D(A)$.

For *b*), let $\psi = (A+i)^{-1}\varphi \in D(A)$. With $A\psi = \varphi - i\psi$ and $U(\varphi) = g^{-1}U(\psi)$, we get

$$(UAU^{-1})(U(\psi)) = U(\varphi) - iU(\psi) = (g^{-1}-i)U(\psi) = f\,U(\psi).$$

Thus, A is unitarily equivalent to multiplication by f. It remains to show that f is real-valued. Since A is self-adjoint, multiplication by f is self-adjoint. If $\mathrm{Im}(f) \neq 0$ μ-a.s., we find a compact set $S \subset \mathbb{C}_+$ with $0 < \mu\big(f^{-1}(S)\big) < \infty$. For the characteristic function $\chi_{f^{-1}(S)}$ associated to this set, this implies $f\chi_{f^{-1}(S)} \in L^2(\Omega, \mathcal{B}(\Omega), \mu)$. Hence, $\mathrm{Im}\langle \chi_{f^{-1}(S)}, f\chi_{f^{-1}(S)}\rangle > 0$. But this is a contradiction, because multiplication by f is self-adjoint. We conclude that f is μ-a.e. real-valued. □

As in the bounded case, Theorem 2.8 enables us to define a measurable functional calculus for bounded, measurable functions $g \in \mathcal{M}(\mathbb{R})$. Given a self-adjoint operator $A : D(A) \to \mathcal{H}$ on a Hilbert space $\mathcal{H}$ and $g \in \mathcal{M}(\mathbb{R})$, we define $g(A) \in \mathcal{L}(\mathcal{H})$ as the multiplication operator that multiplies on $L^2(\Omega, \mathcal{B}(\Omega), \mu)$ by the function

$$Ug(A)U^{-1} = g \circ f$$

where we used the notation of Theorem 2.8. We deduce the following theorem.

Theorem 2.13 (Measurable Functional Calculus, unbounded case)**.** *Let $A : D(A) \to \mathcal{H}$ be self-adjoint. Then there exists a unique linear map $\Psi : \mathcal{M}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ such that*

a) Ψ is an algebraic *-homomorphism.

b) Ψ is bounded with $\|\Psi(g)\|_{\mathcal{L}(\mathcal{H})} \leq \|g\|_\infty$ for all $g \in \mathcal{M}(\mathbb{R})$.

c) Let $(g_n)_{n\in\mathbb{N}}$ a bounded sequence in $\mathcal{M}(\mathbb{R})$ s.t. $|g_n(x)| \leq |x|$ for all $n \in \mathbb{N}$, $x \in \mathbb{R}$ and $\lim_{n\to\infty} g_n(x) = x$ for all $x \in \mathbb{R}$. Then $(\Psi(g_n))_{n\in\mathbb{N}}$ converges strongly *to A.*

d) Let $g \in \mathcal{M}(\mathbb{R})$ and let $(g_n)_{n\in\mathbb{N}}$ be a bounded sequence in $\mathcal{M}(\mathbb{R})$. Assume that g_n converges to g pointwise in $\mathbb{R}$, then $\Psi(g_n)$ converges strongly *to $\Psi(g)$.*

e) If $A\psi = \lambda\psi$ for some $\psi \in D(A), \lambda \in \mathbb{R}$, then $\Psi(g)\psi = f(\lambda)\psi$ for all $g \in \mathcal{M}(\mathbb{R})$.

f) If $g \in \mathcal{M}(\mathbb{R})$ satisfies $g \geq 0$, then $\Psi(g) \geq 0$.

Proof. The existence was explained above and follows from Theorem 2.8. The reader is invited to check properties $a)$ to $f)$. □

We close this section with a remark on the spectral theorem in the so called projection valued measure form. By Theorem 2.13, we have a reasonable definition for the orthogonal projections $\chi_\Omega(A)$ where $\Omega \subset \mathcal{B}(\mathbb{R})$ (here, χ_Ω denotes the characteristic function on the set Ω). Given a vector $\psi \in \mathcal{H}$, the map

$$\mathcal{B}(\mathbb{R}) \ni \Omega \mapsto \langle \psi, \chi_\Omega(A)\psi \rangle \in [0, \infty)$$

defines a positive Borel measure and is interpreted as measuring the probability to find a value of the observable associated to A in the set Ω. The family of operators $\{\chi_\Omega(A) : \Omega \in \mathcal{B}(\mathbb{R})\}$ has the properties that each $\chi_\Omega(A)$ is an orthogonal projection, $\chi_\emptyset(A) = 0$, $\chi_\mathbb{R} = \mathbf{1}_\mathcal{H}$, χ_Ω is the strong limit of $\big(\sum_{i=1}^n \chi_{\Omega_i}(A)\big)_{n\in\mathbb{N}}$ for a disjoint union $\Omega = \cup_{i=1}^\infty \Omega_i$ and finally that $\chi_{\Omega_1}(A)\chi_{\Omega_2}(A) = \chi_{\Omega_1\cap\Omega_2}(A)$. Such a family of operators is called a projection valued measure. Such families of operators are in fact in one-to-one correspondence with self-adjoint operators. This is the content of the spectral theorem in its projection valued measure form which is equivalent to the multiplication operator form discussed above and which gives precise meaning to the formula

$$A = \int_\mathbb{R} \lambda \, \chi_{d\lambda}, \tag{2.18}$$

in close analogy to the finite dimensional spectral theorem. We refer the reader to [55, Theorem VIII.6] as well as the discussion preceeding it for more details on this.

Problem 2.20. *Given a projection valued measure* $\{\chi_\Omega : \Omega \in \mathcal{B}(\mathbb{R})\}$, *explain how to define a densely defined, linear operator* $A : D(A) \to \mathcal{H}$ *through* (2.18) *and show that the resulting operator is self-adjoint. Conversely, given a self-adjoint operator* $A : D(A) \to \mathcal{H}$, *show that it is equal to* (2.18) *for the projection valued measure* $\{\chi_\Omega(A) : \Omega \in \mathcal{B}(\mathbb{R})\}$ *defined through the (unique) measurable functional calculus of* A.

2.5 Applications of the Spectral Theorem

In this section we discuss several applications of the spectral theorem. The main results are the existence of the time evolution of quantum systems, the characterization of the discrete eigenvalues below the essential spectrum of a given self-adjoint operator and the existence and uniqueness of ground state vectors of Schrödinger operators. We also discuss basic results relating self-adjoint operators with symmetric quadratic forms.

2.5.1 Existence of Quantum Dynamics

In quantum mechanics, the time evolution of the system is determined by the time-dependent Schrödinger equation. More precisely, given a self-adjoint Hamilton operator

$A : D(A) \to \mathcal{H}$, a function $t \mapsto \psi(t) \in C(\mathbb{R}; D(A)) \cap C^1(\mathbb{R}; \mathcal{H})$ solves the Schrödinger equation with initial data $\psi_0 \in D(A)$ if

$$\begin{cases} i\partial_t \psi &= A\psi, \\ \psi(0) &= \psi_0. \end{cases} \tag{2.19}$$

The next proposition ensures guarantees the existence of quantum dynamics.

Proposition 2.6. *Let $A : D(A) \to \mathcal{H}$ be self-adjoint and define $U(t) = e^{-itA}$ for $t \in \mathbb{R}$. Then the following holds true.*

a) $(U(t))_{t\in\mathbb{R}}$ is a strongly continuous one-parameter unitary group. That is, $t \mapsto U(t)$ is strongly continuous, $U(t)$ is unitary and $U(t+s) = U(t)U(s)$ for all $t, s \in \mathbb{R}$.

b) If $\psi \in D(A)$, then $\lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi) = -iA\psi$. Conversely, if the limit $\lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi)$ exists for some $\psi \in \mathcal{H}$, then $\psi \in D(A)$.

c) For all $t \in \mathbb{R}$, $U(t)$ leaves $D(A)$ invariant and commutes with A on $D(A)$.

Proof. The proof follows directly from Theorem 2.13 and the corresponding properties of the family of maps $x \mapsto e^{-itx} \in \mathcal{M}(\mathbb{R})$, $t \in \mathbb{R}$. Indeed, let us assume w.l.o.g. that A corresponds to multiplication by f with canonical domain (by the spectral theorem) so that $U(t) = e^{-itf}$. Then *i*) follows directly and for *ii*), we use on the one hand that

$$\frac{1}{t}(e^{-itx} - 1) = -ix \int_0^1 ds\, e^{-itxs},$$

so that $|\frac{1}{t}(e^{-itx} - 1)| \leq |x|$. Combining this with dominated convergence, we conclude that $\lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi) = -iA\psi$ if $\psi \in D(A)$. Conversely, if for some $\varphi \in L^2(d\mu)$

$$\lim_{t\to 0} \|t^{-1}(e^{-itf} - 1)\psi - \varphi\|_2 = 0,$$

then one has pointwise almost sure convergence on a subsequence so that $\varphi = -if\psi \in L^2(d\mu)$, that is $\psi \in D(A)$. Finally, *iii*) follows from the fact that $U(t) = e^{itf}$ commutes with f and $f\varphi \in L^2(d\mu)$ if and only if $e^{itf} f\varphi \in L^2(d\mu)$, for each $t \in \mathbb{R}$. □

Proposition 2.6 shows that that the map $t \mapsto U(t)\psi_0 \in C(\mathbb{R}; D(A)) \cap C^1(\mathbb{R}; \mathcal{H})$ solves the Schrödinger equation (2.19). It is not hard to see that this is the only continuously differentiable solution $\psi \in C(\mathbb{R}; D(A)) \cap C^1(\mathbb{R}; \mathcal{H})$ of the initial value problem (2.19). Indeed, suppose $\psi \in C(\mathbb{R}; D(A)) \cap C^1(\mathbb{R}; \mathcal{H})$ is another solution of (2.19). Then, we can consider $t \mapsto \phi(t) = U(-t)\psi(t) \in C(\mathbb{R}; D(A)) \cap C^1(\mathbb{R}; \mathcal{H})$ with

$$\begin{aligned} \lim_{h\to 0} \frac{1}{h}\big(U(-t-h)\psi(t+h) - U(-t)\psi(t)\big) &= \lim_{h\to 0} \frac{1}{h}\big(U(-t-h) - U(-t)\big)\psi(t) \\ &\quad + \lim_{h\to 0} U(-t-h)\frac{1}{h}\big(\psi(t+h) - \psi(t)\big) \\ &= -AU(-t)\psi(t) + U(-t)(A\psi(t)) = 0, \end{aligned}$$

that is, $\partial_t \phi = 0$ in $\mathcal{H}$. This implies $\phi(t) = \psi_0$ so that $\psi(t) = U(t)\psi_0$ for all $t \in \mathbb{R}$.

The following fundamental structural result shows that every strongly continuous one-parameter unitary group is generated by a self-adjoint operator.

Theorem 2.14 (Stone's Theorem). *Let $(U(t))_{t\in\mathbb{R}}$ be a strongly continuous one-parameter unitary group on a Hilbert space $\mathcal{H}$. Then, there exists a self-adjoint operator $A : D(A) \to \mathcal{H}$ such that $U(t) = e^{-itA}$ for all $t \in \mathbb{R}$.*

Proof. Before defining our candidate for A, we first need to find a suitable dense domain on which we can differentiate $t \mapsto U(t)(\cdot)$. Using that, heuristically, $\phi \approx e^{-itA}\phi$ for small t (assuming we knew the existence of A already), it is useful to consider for $f \in C_c^\infty(\mathbb{R})$ and $\phi \in \mathcal{H}$ the vector space generated by vectors of the form

$$\phi_f = \int_{\mathbb{R}} dt\, f(t)U(t)\phi \in \mathcal{H}.$$

Here, the integral on the r.h.s. can be defined as a vector-valued Riemann integral (and coincides with the usual Bochner integral). Set

$$D = \operatorname{span}(\phi_f : f \in C_c^\infty(\mathbb{R}), \phi \in \mathcal{H}).$$

Then $D \subset \mathcal{H}$ is dense, because for a standard approximation of the identity $(f_n)_{n\in\mathbb{N}}$ in $C_c^\infty(\mathbb{R})$, we have that

$$\|\phi_{f_n} - \phi\|_{\mathcal{H}} = \left\| \int_{\mathbb{R}} dt\, f_n(t)(U(t)\phi - \phi) \right\|_{\mathcal{H}} \leq \sup_{t\,\in\,\operatorname{supp}(f_n)} \|U(t)\phi - \phi\|_{\mathcal{H}} \to 0$$

as $n \to \infty$ (we can choose $\int_{\mathbb{R}} f_n = 1$, $0 \leq f_n \leq 1$, $\operatorname{supp}(f_n) \subset (-1/n; 1/n)$ $\forall\, n \in \mathbb{N}$).

Next, we want to define A (initially on D) through the derivative of $t \mapsto U(t)$. Given $\phi_f \in D$, we compute

$$\begin{aligned}
\lim_{t\to 0} \frac{1}{t}(U(t)\phi_f - \phi_f) &= \lim_{t\to 0} \frac{1}{t} \int_{\mathbb{R}} ds\, f(s)(U(t+s) - U(s))\phi \\
&= \lim_{t\to 0} \frac{1}{t} \int_{\mathbb{R}} ds\, (f(s-t) - f(s))U(s)\phi \\
&= -\int_{\mathbb{R}} f'(s)U(s)\phi = -\phi_{f'},
\end{aligned}$$

where in the last step we applied the dominated convergence theorem. This suggests to define the operator $A : D \to D$ through

$$A\phi_f = i \lim_{t\to 0} \frac{1}{t}(U(t)\phi_f - \phi_f) = -i\phi_{f'}.$$

By definition of the functions $\phi_f \in D$, let us observe that $U(t) : D \to D$ for each $t \in \mathbb{R}$

$(U(t)\phi_f = \phi_{f(.-t)})$, $A : D \to D$ and $[U(t), A] = 0$ in D. A is also symmetric, because

$$\begin{aligned}\langle A\phi_f, \psi_g\rangle_{\mathcal{H}} &= \langle -i\phi_{f'}, \psi_g\rangle_{\mathcal{H}} \\ &= i\int_{\mathbb{R}^2} dsdt\, f'(t)U(-t+s)g(s)\langle\phi,\psi\rangle \\ &= i\int_{\mathbb{R}^2} dsdt\, f'(t)U(s)g(s+t)\langle\phi,\psi\rangle \\ &= -i\int_{\mathbb{R}^2} dsdt\, f(t)U(s)g'(s+t)\langle\phi,\psi\rangle \\ &= \langle\phi_f, A\psi_g\rangle_{\mathcal{H}}.\end{aligned}$$

To finish the proof, we show that A is essentially self-adjoint and that the exponential of its (self-adjoint) closure is equal to $U(t)$. For the first part, suppose that $\psi \in D(A^*)$ with $A^*\psi = i\psi$. Then, for each $\phi \in D$, we compute

$$\partial_t\langle U(t)\phi, \psi\rangle_{\mathcal{H}} = \langle -iAU(t)\phi, \psi\rangle_{\mathcal{H}} = -\langle U(t)\phi, \psi\rangle_{\mathcal{H}}.$$

Solving the ODE, this means that $\langle U(t)\phi, \psi\rangle_{\mathcal{H}} = \langle\phi,\psi\rangle_{\mathcal{H}} e^{-t}$, which implies that $\langle\phi,\psi\rangle_{\mathcal{H}} = 0$, because $e^{-t} \to \infty$ as $t \to -\infty$ while $|\langle -U(t)\phi, \psi\rangle_{\mathcal{H}}| \leq \|\phi\|_{\mathcal{H}}\|\psi\|_{\mathcal{H}}$. Since $\phi \in D$ was arbitrary and $\overline{D} = \mathcal{H}$, this implies that $\psi = 0$. Repeating an analogous argument for the case $A^*\psi = -i\psi$, we deduce that $A : D \to D$ is essentially self-adjoint.

Finally, denote by $\overline{A} : D(\overline{A}) \to \mathcal{H}$ the self-adjoint closure of A and set $V(t) = e^{-it\overline{A}}$. Given $\phi \in D$, we compute that

$$\partial_t\big(U(t)\phi - V(t)\phi\big) = -iAU(t)\phi - i\overline{A}V(t)\phi = -i\overline{A}(U(t) - V(t))\phi,$$

which implies

$$\partial_t\|U(t)\phi - V(t)\phi\|^2_{\mathcal{H}} = 2\,\mathrm{Im}\big\langle\overline{A}(U(t)\phi - V(t)\phi), U(t)\phi - V(t)\phi\big\rangle_{\mathcal{H}} = 0.$$

Thus, $U(t)\phi = V(t)\phi$ for all $t \in \mathbb{R}$ and $\phi \in D$, so that $U(t) = V(t)$, using $\overline{D} = \mathcal{H}$. □

Example 2.20. *Consider the translation group $(U(y))_{y\in\mathbb{R}}$ acting on $L^2(\mathbb{R})$ as*

$$\big(U(y)\psi\big)(x) = \psi(x+y) \ \text{ for a.e. } x \in \mathbb{R},$$

for $\psi \in L^2(\mathbb{R})$. Clearly, $(U(y))_{y\in\mathbb{R}}$ is a strongly continuous unitary group and by Prop. 2.6, $\psi \in \mathcal{H}$ is in the domain $D(A)$ of its generator if and only if

$$\lim_{y\to 0}\frac{1}{y}(U(y) - 1)\psi$$

exists. In this case, the limit equals $-iA\psi$. Comparing this with standard results on Sobolev spaces, we conclude that $D(A) = H^1(\mathbb{R})$ and $U(y) = e^{-iy(i\partial_x)}$. As mentioned before, the observable corresponding to translation of the wave function is momentum.

To view the gradient $i\nabla$ as the generator of translations in $\mathbb{R}^d$, analogously to the previous example, we record the following generalization of Stone's Theorem and we refer to [55, Theorem VIII.12] for its proof.

Theorem 2.15. *Let $\mathbb{R}^d \ni y \mapsto U(y)$ be a strongly continuous map of $\mathbb{R}^d$ into the set of unitary operators on some separable Hilbert space $\mathcal{H}$ and such that*

$$U(y+z) = U(y)U(z) \;\forall\; y,z \in \mathbb{R}^d$$

Set $D = \operatorname{span}\big(\int_{\mathbb{R}^d} dy\, f(y)U(y)\phi \,:\, f \in C_c^\infty(\mathbb{R}^d), \phi \in \mathcal{H}\big)$. Then D is a domain of self-adjointness for each of the generators A_j corresponding to the strongly continuous unitary groups $y_j \mapsto U(0,\dots,0,y_j,0,\dots,0)$, $A_j : D \to D$ and $[A_j, A_k] = 0$ in D. We write in this case $U(y) = e^{iyA} = e^{i\sum_{j=1}^d y_j A_j}$.

2.5.2 Weyl's Criterion and the Min-Max Principle

The Spectral Theorem 2.8 gives us precise information on how general self-adjoint operators look like. In this section, we use this information to characterize the essential and (part of) the discrete spectrum of a general self-adjoint operator. The essential spectrum is described by Weyl's criterion. To describe the part of the discrete spectrum that lies below the essential spectrum, the min-max principle is useful.

Before we start and prove Weyl's criterion, we need the following preparation.

Lemma 2.9. *Let $A_f : D(A_f) \to L^2(\Omega, \mathcal{B}(\Omega), \mu)$ be the self-adjoint multiplication operator on $L^2(\Omega, \mathcal{B}(\Omega), \mu)$ that multiplies with the measurable function $f : \Omega \to \mathbb{R}$ on $D(A_f) = \{\psi \in L^2(\Omega, \mathcal{B}(\Omega), \mu) : f\psi \in L^2(\Omega, \mathcal{B}(\Omega), \mu)\}$. Then*

$$\sigma(A_f) = \big\{\lambda \in \mathbb{R} : \forall \varepsilon > 0 \;\; \textit{we have} \;\; \mu(f^{-1}\big((\lambda-\varepsilon;\lambda+\varepsilon)\big) > 0)\big\} = \text{ess-ran}(f)$$

Proof. We show that $\rho(A_f) \cap \mathbb{R} = \mathbb{R} \setminus \text{ess-ran}(f)$. Indeed, $\lambda \in \mathbb{R} \setminus \text{ess-ran}(f)$ if and only if there exists some $\varepsilon_0 > 0$ such that $\mu(f^{-1}\big((\lambda-\varepsilon_0;\lambda+\varepsilon_0)\big) = 0$. But this means that the measurable function $x \mapsto g_\lambda(x) = (f(x)-\lambda)^{-1}$ is bounded by $|g_\lambda(x)| \le \varepsilon_0^{-1}$ for μ *a.e.* $x \in \Omega$. Hence, the multiplication operator that multiplies by g_λ defines a bounded operator on $L^2(\Omega, \mathcal{B}(\Omega), \mu)$ that inverts $A_f - \lambda$, that is $\lambda \in \rho(A_f)$.

Conversely, if $\lambda \in \rho(A_f) \cap \mathbb{R}$, then the resolvent $(A_f - \lambda)^{-1}$ exists and is bounded. By definition of A_f, the resolvent is equal to multiplication by g_λ. But then, there must exist some $\varepsilon_0 > 0$ such that $\mu(f^{-1}\big((\lambda-\varepsilon_0;\lambda+\varepsilon_0)\big) = 0$: otherwise, we get a contradiction to the boundedness of g_λ by evaluating the norm of $g_\lambda\psi_\varepsilon$ for

$$\psi_\varepsilon = \frac{\chi(f^{-1}\big((\lambda-\varepsilon;\lambda+\varepsilon)\big)}{\mu(f^{-1}\big((\lambda-\varepsilon;\lambda+\varepsilon)\big)} \in L^2(\Omega, \mathcal{B}(\Omega), \mu).$$

Indeed, we have that $\|g_\lambda\psi_\varepsilon\|_2 \ge \varepsilon^{-1}\|\psi_\varepsilon\|_2 = \varepsilon^{-1}$, for each $\varepsilon > 0$. □

Let $A : D(A) \to \mathcal{H}$ be self-adjoint on the Hilbert space $\mathcal{H}$. We call $(\psi_n)_{n\in\mathbb{N}}$ in $D(A)$ a Weyl sequence for A and $\lambda \in \mathbb{R}$ if $\|\psi_n\|_{\mathcal{H}} = 1$ for all $n \in \mathbb{N}$ and $\lim_{n\to\infty} \|(A-\lambda)\psi_n\|_{\mathcal{H}} = 0$.

Theorem 2.16 (Weyl's Criterion)**.** *Let $A : D(A) \to \mathcal{H}$ be self-adjoint. Then $\lambda \in \sigma(A)$ if and only if there exists a Weyl sequence for A and λ. Moreover, $\lambda \in \sigma_{ess}(A)$ if and only if there exists a Weyl sequence for A and λ that converges weakly to zero.*

Proof. Without loss of generality we can consider a multiplication operator A_f on the Hilbert space $\mathcal{H} = L^2(\Omega, \mathcal{B}(\Omega), \mu)$, as in Lemma 2.9.

Assume first that $\lambda \in \sigma(A_f)$. If $\ker(A_f - \lambda) \neq \{0\}$, we can choose $\psi_n = \psi \in \ker(A_f - \lambda)$ for all $n \in \mathbb{N}$ and a fixed, normalized $\psi \in \ker(A_f - \lambda)$ to obtain a Weyl sequence for A and λ. If we assume in addition to $\ker(A_f - \lambda) \neq \{0\}$ that $\lambda \in \sigma_{\mathrm{ess}}(A_f)$, we have either $\dim \ker(A_f - \lambda) = \infty$ or that λ is not isolated in $\sigma(A_f)$. In the first case we can find an orthonormal Weyl sequence of eigenvectors of A_f, which converges weakly to zero. In the second case, we can construct a monotonically decreasing and positive sequence $(\varepsilon_n)_{n\in\mathbb{N}}$ with $\lim_{n\to\infty} \varepsilon_n = 0$ as follows. Defining

$$\Omega_n = f^{-1}\big((\lambda - \varepsilon_n, \lambda + \varepsilon_n)\big)$$

such that $\Omega_{n+1} \subset \Omega_n$, we choose $(\varepsilon_n)_{n\in\mathbb{N}}$ s.t. $\mu(\Omega_n \setminus \Omega_{n+1}) > 0$. Indeed, if for some fixed n_0, $\mu(\Omega_{n_0} \setminus \Omega_{n_0+1}) = 0$ for every choice of $\varepsilon_{n_0+1} > 0$, this would imply that $\mu(f^{-1}\big((\lambda - \varepsilon_{n_0}, \lambda + \varepsilon_{n_0}) \setminus \{\lambda\}\big) = 0$ by monotonicity of μ. This, in turn, would imply that λ is isolated in $\sigma(A)$: for every $\nu \in (\lambda - \varepsilon_{n_0}, \lambda + \varepsilon_{n_0}) \setminus \{\lambda\}$, we can find $\delta > 0$ so that $(\nu - \delta, \nu + \delta) \subset (\lambda - \varepsilon_{n_0}, \lambda + \varepsilon_{n_0}) \setminus \{\lambda\}$ so that $\mu(f^{-1}(\nu - \delta, \nu + \delta)) = 0$ and thus $\sigma(A_f) \cap ((\lambda - \varepsilon_{n_0}, \lambda + \varepsilon_{n_0}) \setminus \{\lambda\}) = \emptyset$. But we excluded in the beginning that λ is isolated. Hence, let us choose $(\varepsilon_n)_{n\in\mathbb{N}}$ as claimed, then the sequence $(\psi_n)_{n\in\mathbb{N}}$ defined by

$$\psi_n = \|\chi_{\Omega_n \setminus \Omega_{n+1}}\|_2^{-1} \chi_{\Omega_n \setminus \Omega_{n+1}} \in D(A_f)$$

is an orthonormal Weyl sequence due to $\|(A - \lambda)\psi_n\| \leq \varepsilon_n \to 0$ as $n \to \infty$. Since it is an orthonormal sequence, it also converges weakly to zero. Next, assume that $\lambda \in \sigma(A_f)$ and $\ker(A_f - \lambda) = \{0\}$ so that $\lambda \in \sigma_{\mathrm{ess}}(A_f)$. Note that λ is not isolated in this case (*why?*). Thus, we can repeat the previous argument and choose Ω_n and ψ_n, $n \in \mathbb{N}$ to find a Weyl sequence that converges weakly to zero.

In summary, we have proved that $\lambda \in \sigma(A_f)$ implies that there exists a Weyl sequence for A_f and λ and that the sequence converges weakly to zero if $\lambda \in \sigma_{\mathrm{ess}}(A_f)$.

Conversely, assume that $(\psi_n)_{n\in\mathbb{N}}$ is a Weyl sequence for A_f and λ. Then, we claim that λ can not lie in $\rho(A_f)$. In fact, if we assume that $\lambda \in \rho(A_f)$, then $(A - \lambda)^{-1} : \mathcal{H} \to D(A_f)$ is bounded. But this yields a contradiction, because

$$1 = \|\psi_n\|_2 \leq \|R_\lambda(A_f)\|_{\mathcal{L}(\mathcal{H})} \|(A_f - \lambda)\psi_n\|_2 \to 0 \quad (n \to \infty).$$

Finally, if the Weyl sequence converges weakly to zero, we claim that $\lambda \notin \sigma_{\mathrm{d}}(A_f)$. Indeed, assuming that $\lambda \in \sigma_{\mathrm{d}}(A_f)$, let us denote by P_λ the orthogonal projection onto the finite dimensional subspace $\ker(A_f - \lambda)$. Notice that P_λ is equal to the operator that multiplies by $\chi_{f^{-1}(\{\lambda\})}$ (this is true for all eigenvalues λ of A, independently of their multiplicity): if $A_f\psi = f\psi = \lambda\psi$, ψ must have support in $f^{-1}(\{\lambda\})$, so that

$$\ker(A_f - \lambda) = \big\{\chi_{f^{-1}(\{\lambda\})}\psi : \psi \in D(A_f)\big\}.$$

Now let $P_\lambda^\perp = \mathbf{1} - P_\lambda$, then the previous observation and the assumption that λ is an isolated point in the spectrum imply that

$$(P_\lambda^\perp \psi)(x) = \chi_{\mathbb{R}\setminus f^{-1}(\{\lambda\})}(x)\psi(x) = \chi_{\mathbb{R}\setminus f^{-1}((\lambda-\delta;\lambda+\delta))}(x)\psi(x) \tag{2.20}$$

$\mu - a.s.$ for some $\delta > 0$. Indeed, for $\varepsilon > 0$ small enough, we know that

$$\sigma(A_f) \cap (\lambda - \varepsilon; \lambda + \varepsilon) \setminus \{\lambda\} = \emptyset.$$

Using the characterization $\sigma(A_f) = \text{ess-ran}(f)$, a standard compactness argument and the subadditivity of μ, this shows that

$$\mu\big(f^{-1}\big([\lambda - \delta', \lambda - \varepsilon'] \cup [\lambda + \varepsilon', \lambda + \delta']\big)\big) = 0$$

for suitable $\delta' > 0$ fixed and for every $\varepsilon' > 0$ sufficiently small. By continuity of μ, this yields $\mu(f^{-1}\ ([\lambda - \delta', \lambda + \delta'] \setminus \{\lambda\})) = 0$ and thus (2.20).

From (2.20), we conclude that for all $n \in \mathbb{N}$, we have that

$$\|(A_f - \lambda)P_\lambda^\perp \psi_n\|_2 \geq \delta \|P_\lambda^\perp \psi_n\|$$

and therefore

$$\lim_{n\to\infty} \|P_\lambda^\perp \psi_n\| \leq \delta^{-1} \lim_{n\to\infty} \|(A_f - \lambda)P_\lambda^\perp \psi_n\|_2 \leq \delta^{-1} \lim_{n\to\infty} \|(A_f - \lambda)\psi_n\|_2 = 0.$$

Now, P_λ projects onto a finite dimensional space and $(P_\lambda \psi_n)_{n\in\mathbb{N}}$ is a bounded sequence, $\|P_\lambda \psi_n\| \leq 1$ for all $n \in \mathbb{N}$: it has in particular a strongly convergent subsequence. Since $(P_\lambda^\perp \psi_n)_{n\in\mathbb{N}}$ converges strongly to zero, this means that $(\psi_n)_{n\in\mathbb{N}}$ has a strongly convergent subsequence and its limit must be zero, since $(\psi_n)_{n\in\mathbb{N}}$ converges weakly to zero, by assumption. But $\|\psi_n\|_2 = 1$ for all $n \in \mathbb{N}$, a contradiction. Given a Weyl sequence weakly converging to zero, we must therefore have $\lambda \in \sigma_{\text{ess}}(A_f)$. □

Remark. Observe that the proof implies that for $\lambda \in \sigma_{\text{ess}}(A)$, we find an orthonormal, and consequently weakly convergent, Weyl sequence for A and λ.

Problem 2.21. *Consider the self-adjoint operators $-\Delta : H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^2)$ and $|X|^2 = A_f : D(A_f) \to L^2(\mathbb{R}^d)$ for $f(x) = |x|^2$. Prove that $\sigma(-\Delta) = \sigma_{\text{ess}}(-\Delta)$ and $\sigma(|X|^2) = \sigma_{\text{ess}}(|X|^2)$. Determine in both cases the spectrum explicitly.*

Weyl's criterion characterizes the essential spectrum of a self-adjoint operator. This part of the spectrum is closely related to the concept of asymptotic completeness in scattering theory; see [57] for a thorough discussion. In the many-body examples discussed in these notes, on the other hand, we are primarily interested in situations where the Hamiltonian has purely discrete spectrum and a fundamental task in quantum mechanics is then to determine the different energy levels, that is the eigenvalues of the Hamiltonian. Since an exact calculation of the spectrum is in general out of reach, one needs methods to approximate the eigenvalues. A particularly useful criterion to estimate eigenvalues is the Min-Max Principle.

Theorem 2.17 (Min-Max Principle)**.** *Let $A : D(A) \to \mathcal{H}$ be self-adjoint and such that $\langle\psi, A\psi\rangle_{\mathcal{H}} \geq C\|\psi\|^2_{\mathcal{H}}$ for all $\psi \in D(A)$ and some $C \in \mathbb{R}$. Define $\lambda_k \in \mathbb{R}$, $k \in \mathbb{N}$, by*

$$\lambda_k = \inf_{\substack{V \subset D(A),\\ \dim(V)=k}} \max_{\substack{\psi\in V,\\ \|\psi\|_{\mathcal{H}}=1}} \langle\psi, A\psi\rangle$$

such that $(\lambda_k)_{k\in\mathbb{N}}$ is a monotonically increasing sequence and bounded below by C. Then

i) The following holds true for every $k \in \mathbb{N}$: we have that $\lambda_k \in \sigma(A)$ and if there exists some $j \geq k$ such that $\lambda_j < \lambda_{j+1}$, then $\lambda_1, \dots, \lambda_k$ are discrete eigenvalues of A, counted with multiplicity.

ii) We have that $E_0 = \inf \sigma_{ess}(A) = \lim_{k\to\infty} \lambda_k$ and the spectrum below E_0 is given by $\sigma(A) \cap (-\infty; E_0) = \{\lambda_k : k \in \mathbb{N}\} \cap (-\infty; E_0)$. In particular, if $E_0 = \infty$, then $\sigma(A) = \sigma_d(A) = \{\lambda_k : k \in \mathbb{N}\}$ and $\sigma_{ess}(A) = \emptyset$.

Remarks:

1) In the context of quantum mechanics, the first min-max value $\lambda_1 = \inf_{\psi\in D(A),\|\psi\|_{\mathcal{H}}=1}\langle\psi, A\psi\rangle$ is called the ground state energy of the Hamiltonian A. It describes the lowest possible energy the system can have.

2) Let $A : D \to \mathcal{H}$ and $B : D \to \mathcal{H}$ be self-adjoint and suppose that $A \leq B$. Denote by $(\lambda_k)_{k\in\mathbb{N}}$ the min-max values of A and by $(\mu_j)_{j\in\mathbb{N}}$ those of B. Then $\lambda_k \leq \mu_k$ for all $k \in \mathbb{N}$.

Corollary 2.5. *If $\lambda_k \to \infty$ as $k \to \infty$, then there exists an orthonormal eigenbasis of A and $(A - C + 1)^{-1} : \mathcal{H} \to D(A) \subset \mathcal{H}$ is a compact operator.*

Proof. By the spectral theorem and the min-max theorem, we have a spectral decomposition of A into the countable sum

$$A = \sum_{k=1}^{\infty} \lambda_k |\varphi_k\rangle\langle\varphi_k| \tag{2.21}$$

for an orthonormal sequence $(\varphi_k)_{k\in\mathbb{N}}$ of eigenvectors of A. Indeed, by the spectral theorem, we can assume that A corresponds to multiplication by some $f : \Omega \to \mathbb{R}$ on a measure space $(\Omega, \mathcal{B}(\Omega), \mu)$. The spectrum $\sigma(A)$ of A is the essential range of f and by assumption, it is purely discrete, $\sigma(A) = \sigma_{\mathrm{d}}(A)$. By definition of the essential range, one can verify with a simple covering argument that $\mu(f^{-1}(\mathbb{R} \setminus \sigma_{\mathrm{d}}(A))) = 0$ so that

$$f(x) = \sum_{\lambda\in\sigma_{\mathrm{d}}(A)} f(x)\chi_{f^{-1}(\{\lambda\}}(x) = \sum_{\lambda\in\sigma_{\mathrm{d}}(A)} \lambda\, \chi_{f^{-1}(\{\lambda\}}(x) \quad \text{for} \quad \mu - a.e.\ x \in \Omega.$$

Since the eigenspace $\mathrm{Eig}(\lambda_k)$ of A for λ_k is finite dimensional and equal to

$$\mathrm{Eig}(\lambda_k) = \big\{\psi \in L^2(d\mu) : \psi = \psi\chi_{f^{-1}(\{\lambda_k\}}\ \ \mu - a.s.\big\},$$

we obtain the representation (2.21). Analogously, for any $\psi \in L^2(d\mu)$, we have that

$$\psi(x) = \sum_{\lambda \in \sigma_{\mathrm{d}}(A)} \psi(x)\, \chi_{f^{-1}(\{\lambda\})}(x) \quad \text{for} \quad \mu - a.e.\ x \in \Omega,$$

so that the $(\varphi_k)_{k\in\mathbb{N}}$ form an orthonormal basis, that is $\mathcal{H} = \overline{\operatorname{span}(\varphi_k : k \in \mathbb{N})}$.

For the compactness of $(A - C + 1)^{-1}$, we use the spectral decomposition

$$(A - C + 1)^{-1} = \sum_{k=1}^{\infty} (\lambda_k - C + 1)^{-1} |\varphi_k\rangle\langle\varphi_k|.$$

If $(\psi_n)_{n\in\mathbb{N}}$ is a sequence in $\mathcal{H}$ such that $\|\psi_n\|_{\mathcal{H}} \leq 1$ for all $n \in \mathbb{N}$, then for some subsequence $\psi_{n_j} \rightharpoonup \psi \in \mathcal{H}$ as $j \to \infty$ for some weak limit $\psi \in \mathcal{H}$. In particular, we obtain that $|\langle \psi_{n_j}, \varphi_k\rangle_{\mathcal{H}}|^2 \to |\langle \psi, \varphi_k\rangle_{\mathcal{H}}|^2$ for every fixed $k \in \mathbb{N}$. But then

$$\begin{aligned}
\Big\| \frac{1}{A - C + 1} (\psi_{n_j} - \psi) \Big\|_{\mathcal{H}}^2 &\leq \sum_{k \geq k_0} \frac{|\langle \psi_{n_j} - \psi, \varphi_k\rangle_{\mathcal{H}}|^2}{(\lambda_{k_0} - C + 1)^2} + \sum_{k < k_0} \frac{|\langle \psi_{n_j} - \psi, \varphi_k\rangle_{\mathcal{H}}|^2}{(\lambda_k - C + 1)^2} \\
&\leq \frac{4}{(\lambda_{k_0} - C + 1)^2} + \sum_{k < k_0} \frac{|\langle \psi_{n_j} - \psi, \varphi_k\rangle_{\mathcal{H}}|^2}{(\lambda_k - C + 1)^2} \to \frac{4}{(\lambda_{k_0} - C + 1)^2}
\end{aligned}$$

as $j \to \infty$. Since $\lambda_{k_0} \to \infty$ as $k_0 \to \infty$, this implies the compactness of $(A - C + 1)^{-1}$. $\square$

Proof of Theorem 2.17. *i)* We proceed by induction and start with the case $k = 1$. We claim that $\lambda_1 = \inf \sigma(A) \in \sigma(A)$. Indeed, A is bounded from below by λ_1 and therefore $\sigma(A) \subset [\lambda_1, \infty)$. On the other hand, $\lambda_1 \in \sigma(A)$: if A corresponds to multiplication by f in $L^2(d\mu)$, via the spectral theorem, then λ_1 must be in the essential range of f, because otherwise $\mu(f^{-1}(\lambda_1 - \varepsilon, \lambda_1 + \varepsilon)) = 0$ for some $\varepsilon > 0$ which would imply $A \geq \lambda_1 + \varepsilon$ (a contradiction to the definition of λ_1).

Now, assume $\lambda_1 \in \sigma_{\mathrm{ess}}(A)$. Then we can find an orthonormal Weyl sequence $(\psi_n)_{n\in\mathbb{N}}$ for λ_1, as in the proof of Weyl's criterion. Choosing a suitable subsequence, we find for every $j \geq 1$ and $\delta > 0$ a $(j + 1)$-dimensional subspace

$$V = \operatorname{span}(\psi_{n_l} : l = 1, \ldots, j + 1)$$

on which

$$\langle \psi, A\psi\rangle_{\mathcal{H}} \leq \lambda_1 + \delta$$

for every $\psi \in V$ with $\|\psi\|_{\mathcal{H}} = 1$. Indeed, given $\delta > 0$, we choose the n_l so large s.t.

$$\|(A - \lambda_1)\psi_{n_l}\| < \frac{\delta}{\sqrt{j+1}}.$$

For a normalized vector $\psi = \sum_{l=1}^{j+1} \alpha_l \psi_{n_l}$ with $1 = \|\psi\|^2 = \sum_{l=1}^{j+1} |\alpha_l|^2$, this implies

$$|\langle \psi, A\psi\rangle_{\mathcal{H}} - \lambda_1| \leq \max_{s=1,\ldots,j+1} \|(A - \lambda_1)\psi_{n_s}\| \sum_{l=1}^{j+1} |\alpha_l| < \delta.$$

The existence of such a subspace implies that

$$\lambda_1 \leq \lambda_{j+1} \leq \sup_{\psi \in V : \|\psi\|_{\mathcal{H}}=1} \langle \psi, A\psi \rangle_{\mathcal{H}} \leq \lambda_1 + \delta.$$

Since $\delta > 0$ was arbitrary, we conclude that $\lambda_1 = \lambda_{j+1}$ for every $j \leq 1$. By contraposition, if there exists $j \geq 1$ such that $\lambda_1 < \lambda_{j+1}$, we must have $\lambda_1 \in \sigma_{\mathrm{d}}(A)$.

Consider now the inductive step. If $\lambda_{k+1} = \lambda_k$, then $\lambda_{k+1} \in \sigma(A)$. If $\lambda_k < \lambda_{k+1}$, then $\lambda_1, \ldots, \lambda_k$ are discrete eigenvalues of A counted with multiplicity, by the inductive assumption. Similarly, if we assume $\lambda_j < \lambda_{j+1}$ for some $j \geq k+1$, the inductive assumption implies that $\lambda_1, \ldots, \lambda_k$ are eigenvalues of A counted with multiplicity. In each of the two cases, this means that we find $V_k = \operatorname{span}(\varphi_1, \ldots, \varphi_k)$ a k-dimensional subspace in $D(A)$ spanned by orthonormal eigenvectors corresponding to the first k min-max values $\lambda_1, \ldots, \lambda_k$. We then define the operator

$$A^{(k)} = (A)_{|D(A)\cap V_k^{\perp}} : D(A) \cap V_k^{\perp} \to \mathcal{H} \cap V_k^{\perp}$$

and check as an exercise that $A^{(k)}$ is self-adjoint as an operator acting on a dense domain in $\mathcal{H} \cap V_k^{\perp}$ (the key observation is that A leaves V_k and $V_k^{\perp}$ invariant). Now, we claim that the min-max values $(\nu_i)_{i\in\mathbb{N}}$ of $A^{(k)}$ satisfy $\nu_i = \lambda_{k+i}$ for every $i \in \mathbb{N}$.

We verify this for ν_1 - the general case is left as an exercise. To show that $\nu_1 = \lambda_{k+1}$ let us first exclude that $\nu_1 < \lambda_{k+1}$. For if $\nu_1 < \lambda_{k+1}$, just pick some normalized vector $\varphi_{k+1} \in V_k^{\perp}$ with $\langle \varphi, A\varphi \rangle_{\mathcal{H}} < \lambda_{k+1}$. If $\lambda_k < \lambda_{k+1}$, this yields a contradiction to the definition of λ_{k+1} by controlling A in form sense on the $(k+1)$-dimensional subspace $\operatorname{span}(V_k \cup \{\varphi\}) \subset \mathcal{H}$. Recall here that for a vector $\sum_{j=1}^{k} \alpha_j \psi_j + \beta\varphi_{k+1}$, we have

$$\left\langle \sum_{j=1} \alpha_j \psi_j + \beta\varphi_{k+1}, A\Big(\sum_{j=1} \alpha_j \psi_j + \beta\varphi_{k+1} \Big) \right\rangle = \sum_{j=1}^{k} \lambda_j |\alpha_j|^2 + \beta^2 \langle \varphi_{k+1}, A\varphi_{k+1} \rangle,$$

by orthonormality. Thus, we have $\nu_1 \geq \lambda_{k+1}$ and we can also exclude that $\nu_1 > \lambda_{k+1}$. For if the latter was true, there must exist some normalized $\varphi \in V_k^{\perp}$ with $\langle \varphi, A\varphi \rangle_{\mathcal{H}} < \nu_1$, contradicting the definition of ν_1. The existence of such a φ follows by observing that $\nu_1 > \lambda_{k+1}$ implies that we find a $(k+1)$-dimensional subspace W_{k+1} on which

$$\langle \psi, A\psi \rangle_{\mathcal{H}} \leq \lambda_{k+1} + \delta < \nu_1$$

for normalized $\psi \in W_{k+1}$ and small $\delta > 0$, by definition of λ_{k+1}. If $P_k : W_{k+1} \to V_k$ denotes the orthogonal projection into V_k, then $k+1 = \dim\ker(P_k) + \dim\operatorname{ran}(P_k)$, where $\dim\operatorname{ran}(P_k) \leq k$ and where $\ker(P_k) \subset V_k^{\perp}$, hence the claim.

In conclusion, $\nu_1 = \lambda_{k+1} \in \sigma(A^{(k)})$, by the inductive assumption. Hence, by the characterization of $\sigma(A)$ through Weyl sequences and by definition of $A^{(k)}$, we conclude $\lambda_{k+1} \in \sigma(A)$. If in addition $\lambda_j < \lambda_{j+1}$ for some $j \geq k+1$, then this means that $\nu_j < \nu_{j+1}$ for some $j \geq 1$ (by $\lambda_{k+i} = \nu_i$), and the inductive assumption implies that ν_1 is an eigenvalue of $A^{(k)}$ so that λ_{k+1} is an eigenvalue of A and we find an eigenfunction in $V_k^\perp$. This means that $\lambda_1, \dots, \lambda_{k+1}$ are eigenvalues of A counted with multiplicity and it concludes the inductive step. This proves i).

ii) Let's start to prove that $\lambda_k \leq E_0$ for all $k \in \mathbb{N}$. We may assume that $E_0 < \infty$, otherwise there is nothing to prove. Since $\sigma_{\mathrm{d}}(A)$ consists of isolated eigenvalues of A, $\sigma_{\mathrm{ess}}(A)$ is closed (*exercise*) and hence $E_0 \in \sigma_{\mathrm{ess}}(A)$. From the proof of Theorem 2.16, we find an orthonormal Weyl-sequence $(\psi_n)_{n\in\mathbb{N}}$ with $\|\psi_n\|_2 = 1$ for all $n \in \mathbb{N}$ s.t.

$$\lim_{n\to\infty} |\langle \psi_n, (A - E_0)\psi_n\rangle| \leq \lim_{n\to\infty} \|(A - E_0)\psi_n\|_2 = 0.$$

Choosing for small $\delta > 0$, as in the proof of *i*), a suitable finite subsequence $(\psi_n)_{n_0 \leq n \leq N_0}$ for sufficiently large $n_0, N_0 \in \mathbb{N}$, we conclude

$$\lambda_k \leq E_0 + \max_{\substack{\psi\in\mathrm{span}(\{\psi_n : n_0 \leq n \leq N_0\}),\\ N_0 - n_0 \geq k, \|\psi\|_2 = 1}} \langle \psi, (A - E_0)\psi\rangle \leq E_0 + \delta$$

Hence, $\lambda_k \leq E_0$ for all $k \in \mathbb{N}$. Note that trivially $\lambda_k \in \sigma_{\mathrm{d}}(A)$ if $\lambda_k < E_0$.

Now let us prove that $\lambda_\infty = \lim_{k\to\infty} \lambda_k = E_0$. If $\lambda_\infty < E_0$, then $\lambda_\infty \in \sigma_{\mathrm{d}}(A)$ (note that $\lambda_\infty \in \sigma(A)$ by closedness of the spectrum). In particular, λ_∞ is isolated so that $(\lambda_k)_{k\in\mathbb{N}}$ must be constant, up to finitely many terms. Assume w.l.o.g. that $\lambda_k = \lambda_\infty$ for all $k \in \mathbb{N}$. As in *i*), we restrict A to $U = \mathrm{Eig}(\lambda_\infty)^\perp$ and conclude that $\nu_1 = \lambda_{\dim(\mathrm{Eig}(\lambda_\infty))+1} = \lambda_\infty \in \sigma(A_{|U})$. Now, $\lambda_\infty \notin \sigma_{\mathrm{ess}}(A_{|U}) \subset \sigma_{\mathrm{ess}}(A)$, but this means we find an eigenvector of A in the orthogonal complement of $\mathrm{Eig}(\lambda_\infty)$, a contradiction.

Finally, let's prove that $\{\lambda_k : k \in \mathbb{N}\} \cap (-\infty, E_0) = \sigma(A) \cap (-\infty, E_0)$. Part *i*) and the arguments from above show that $\{\lambda_k : k \in \mathbb{N}\} \subset \sigma(A) \cap (-\infty, E_0]$. Conversely, let $\mu \in \sigma(A) \cap (-\infty, E_0)$. This means by definition of E_0 that $\mu \in \sigma_{\mathrm{d}}(A)$. What we need to show is that $\mu \in \sigma_{\mathrm{d}}(A)$ implies that μ is equal to some $\lambda_k < E_0$. We certainly have $\mu \geq \lambda_1$ and $\mu \leq \lambda_{k_0}$ for some $k_0 \in \mathbb{N}$, because $\mu < \lim_{k\to\infty} \lambda_k = E_0$. Then either $\mu \in \{\lambda_1, \dots, \lambda_{k_0}\}$ or there are min-max values $\lambda_l < \mu < \lambda_{l+1}$. But the latter contradicts the definition of λ_{l+1} by evaluating A in form sense in the $(l+1)$-dimensional space formed by the orthonormal eigenvectors related to the eigenvalues $\lambda_1, \dots, \lambda_l$ and μ. □

Problem 2.22. *Prove that $A^{(k)}$ is self-adjoint and that $\nu_i = \lambda_{k+i}$, $\forall\, i \in \mathbb{N}$.*

The Weyl criterion and the Min-Max Principle are quite useful tools for studying the spectrum of a self-adjoint operator. One consequence is the discreteness of the spectrum of Hamiltonians with trapping potentials. The picture is that a potential that grows to infinity as $|x| \to \infty$ makes it impossible for the particles to escape to infinity, that is, they are effectively trapped in some finite region $\Omega \subset \mathbb{R}^d$.

Corollary 2.6. *Let $H = -\Delta + V : D(H) \to L^2(\mathbb{R}^d)$ be self-adjoint, where $V \in L^\infty_{loc}(\mathbb{R}^d)$ is a locally bounded potential satisfying $V(x) \to \infty$ as $|x| \to \infty$. Then, the min-max values $\lambda_k(H)$ of H satisfy $\lambda_k(H) \to \infty$ as $k \to \infty$ and $\sigma_{ess}(H) = \emptyset$.*

Remark 2.1. *Recall from Proposition 2.5 that $\overline{H_{|C_c^\infty(\mathbb{R}^d)}}$ is self-adjoint.*

Remark 2.2. *The corollary implies $\sigma(-\Delta + |X|^2) = \sigma_{\mathrm{d}}(-\Delta + |X|^2)$ (cf. Problem 2.21).*

Proof. Assume w.l.o.g. that $V \geq 0$ and denote by $(\lambda_k)_{k\in\mathbb{N}}$ the min-max values of H. We assume by contradiction that $\lim_{k\to\infty} \lambda_k = \lambda_\infty = \inf \sigma_{\text{ess}}(-\Delta + V) < \infty$. By Theorem 2.16, there exists a Weyl sequence $(\psi_n)_{n\in\mathbb{N}}$ for H and λ_∞ that converges weakly to zero. In particular, we have that

$$\lim_{n\to\infty} \left[\int_{\mathbb{R}^d} dx\, \left[|\nabla\psi_n(x)|^2 + V(x)|\psi_n(x)|^2 \right] - \lambda_\infty \right] = 0.$$

This implies that $(\psi_n)_{n\in\mathbb{N}}$ is bounded in $H^1(\mathbb{R}^d)$. Now fix some $R > 0$ and denote by $\varphi_R \in C_c^\infty(B_R(0)) \subset C_c^\infty(\mathbb{R}^d)$ a smooth, compactly supported and non-negative function which is bounded by one and which is s.t. $\varphi_R(x) = 0$ for all $|x| > 2R$ and $\varphi_R(x) = 1$ if $|x| \leq R/2$. We consider $(\psi_n\varphi_R)_{n\in\mathbb{N}}$ in $H^1(\mathbb{R}^d)$ and conclude from the Rellich-Kondrashov compactness theorem (see e.g. [40, Theorem 8.9]) that $(\psi_n\varphi_R)_{n\in\mathbb{N}}$ has a strongly convergent subsequence in $L^2(\mathbb{R}^d)$, denoted again by $(\psi_n\varphi_R)_{n\in\mathbb{N}}$. Since the weak limit of $(\psi_n)_{n\in\mathbb{N}}$ in $L^2(\mathbb{R}^d)$ is zero, we must have $\lim_{n\to\infty} \psi_n\varphi_R = 0$ in $L^2(\mathbb{R}^d)$. But we also have that

$$\int_{\mathbb{R}^d} dx\, (1 - \varphi_R)|\psi_n(x)|^2 \leq \frac{\int_{\mathbb{R}^d} dx\, V(x)|\psi_n(x)|^2}{\inf_{|x|\geq R/2} V(x)} \leq \frac{C}{\inf_{|x|\geq R/2} V(x)}$$

for some constant $C > 0$ which is independent of $n \in \mathbb{N}$. Choosing first $R > 0$ and then $n \in \mathbb{N}$ sufficiently large, shows that $1 = \|\psi_n\|_2 \to 0$ as $n \to \infty$: a contradiction. As a consequence, we conclude that $\inf \sigma_{\text{ess}}(-\Delta + V) = \infty$, that is $\sigma_{\text{ess}}(-\Delta + V) = \emptyset$. $\square$

2.5.3 Existence and Uniqueness of Ground States

We have seen in Corollary 2.6 that Hamiltonians with trapping potentials have purely discrete spectrum. In this section, we use the functional calculus to show that the ground state energy of such Hamiltonians is non-degenerate and that the ground state vector can be chosen to be strictly positive. The result is sometimes also useful for proving the uniqueness of minimizers of nonlinear functionals as illustrated in the next chapter.

Throughout this section, we work in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d)$. We begin with an abstract result which provides a strategy to prove the uniqueness and positivity of eigenfunctions of Schrödinger operators. Sometimes this is referred to as the Perron-Frobenius principle, in analogy to the well-known result from linear algebra. To state and prove the theorem, we need to introduce some notation: $f \in L^2(\mathbb{R}^d)$ is called positive if $f(x) > 0$ for *a.e.* $x \in \mathbb{R}^d$ (it is called non-negative if $f(x) \geq 0$ for *a.e.* $x \in \mathbb{R}^d$). If f is positive (non-negative), we write $f > 0$ ($f \geq 0$). A bounded operator $A \in \mathcal{L}(\mathcal{H})$ is called positivity preserving if $Af \geq 0$ with $Af \not\equiv 0$ whenever $f \geq 0$ with $f \not\equiv 0$ and it is called positivity improving if $f \geq 0$ with $f \not\equiv 0$ implies that $Af > 0$ is positive. Finally, $A \in \mathcal{L}(\mathcal{H})$ is called real if it maps real functions to real functions. Notice that a positivity improving operator is real: if $\psi = \psi_+ - \psi_-$ is real and split into its positive and negative parts, then $A\psi = A\psi_+ - A\psi_-$ and both $A\psi_+, A\psi_- \geq 0$. In particular, they are real valued, so $A\psi$ is real.

Proposition 2.7. *Let $A \in \mathcal{L}(\mathcal{H})$ be a self-adjoint and positivity improving operator. Then, if $\lambda = \|A\|_{\mathcal{L}(\mathcal{H})}$ is an eigenvalue of A, it is simple and the corresponding normalized eigenvector can be chosen to be positive.*

Proof. Let $\psi \in \mathcal{H}$ denote a normalized eigenvector of A s.t. $A\psi = \lambda\psi$. Since A maps real functions to real functions, the real and imaginary parts of ψ are also eigenvectors of A with eigenvalue λ. Therefore, assume w.l.o.g. that ψ is real-valued and normalized. We can decompose ψ into the sum of its positive and negative parts, $\psi = \psi_+ - \psi_-$ where $\psi_+ = \max(\psi, 0)$ and $\psi_- = \max(-\psi, 0)$. We claim that $\langle \psi, A\psi\rangle_{\mathcal{H}} = \langle |\psi|, A|\psi|\rangle_{\mathcal{H}}$. Indeed, this follows from

$$\lambda = \langle \psi, A\psi\rangle_{\mathcal{H}} \leq \langle |\psi|, |A\psi|\rangle_{\mathcal{H}} = \langle |\psi|, |A\psi_+ - A\psi_-|\rangle_{\mathcal{H}} \leq \langle |\psi|, A|\psi|\rangle_{\mathcal{H}} \leq \|A\|_{\mathcal{L}(\mathcal{H})} = \lambda$$

where we used that $|\psi| = \psi_+ + \psi_-$. Thus $\langle \psi, A\psi\rangle_{\mathcal{H}} = \langle |\psi|, A|\psi|\rangle_{\mathcal{H}}$ and we find that

$$\langle \psi_+, A\psi_-\rangle_{\mathcal{H}} = \frac{1}{4}\langle (|\psi| + \psi), A(|\psi| - \psi)\rangle_{\mathcal{H}} = \frac{1}{4}\langle |\psi|, A|\psi|\rangle_{\mathcal{H}} - \frac{1}{4}\langle \psi, A\psi\rangle_{\mathcal{H}} = 0.$$

Since A is positivity improving and the inner product of a non-negative, not identically vanishing function with a positive function is positive, we conclude that either $\psi = \psi_+$ or $\psi = \psi_-$. Let's assume for definiteness that $\psi = \psi_+$ and $\psi_- = 0$. Then, this implies $\psi = \|A\|^{-1}_{\mathcal{L}(\mathcal{H})} A\psi > 0$. Hence, every real eigenfunction of A with eigenvalue λ is positive, up to multiplication by a constant. If we assume that there are two different real eigenfunctions ψ_1, ψ_2 with eigenvalue λ, we may assume w.l.o.g. that they are orthogonal, but two positive functions in $L^2(\mathbb{R}^d)$ are never orthogonal. We conclude that λ is simple and we can choose the eigenvector to be positive. □

Proposition 2.7 is a statement about bounded self-adjoint operators. Of course, the operators that we typically analyze are not bounded. However, as already used in the proof of the spectral theorem, we can also obtain information about the ground state vector of a self-adjoint operator by considering its resolvent.

Proposition 2.8. *Let $A : D(A) \to \mathcal{H}$ be self-adjoint operator so that $\lambda = \inf \sigma(A) \in \mathbb{R}$ is an eigenvalue of A (in particular $A \geq \lambda$ is semi-bounded). Assume moreover that*

$$\left\{e^{-tA} : t \in [0, \infty)\right\} \subset \mathcal{L}(\mathcal{H})$$

is a family of positivity improving operators. Then, λ_0 is a simple eigenvalue of A and the corresponding eigenvector is positive, after multiplication by a constant phase.

Proof. Let $\mu < \lambda$. An application of the spectral theorem 2.8 proves the useful formula

$$\langle \psi, (A-\mu)^{-1}\varphi\rangle_{\mathcal{H}} = \int_0^\infty \langle \psi, e^{-(A-\mu)t}\varphi\rangle_{\mathcal{H}}\, dt = \int_0^\infty e^{\mu t}\langle \psi, e^{-At}\varphi\rangle_{\mathcal{H}}\, dt \tag{2.22}$$

for all $\psi, \varphi \in \mathcal{H}$. Fixing $\varphi \geq 0$, the assumption on $\left\{e^{-tA} : t \in [0, \infty)\right\} \subset \mathcal{L}(\mathcal{H})$ and (2.22) show that $(A-\mu)^{-1} \in \mathcal{L}(\mathcal{H})$ is positivity improving, because $\psi \geq 0$ is arbitrary. Now, if ψ is an eigenvector of A with eigenvalue λ, then ψ is also an eigenvector of $(A-\mu)^{-1}$ with eigenvalue $(\lambda-\mu)^{-1}$. But we have for any $\varphi \in \mathcal{H}$ that

$$0 \leq \langle \varphi, (A-\mu)^{-2}\varphi\rangle_{\mathcal{H}} \leq (\lambda_0-\mu)^{-1}\langle \varphi, (A-\mu)^{-1})\varphi\rangle_{\mathcal{H}} \leq (\lambda-\mu)^{-2}\|\varphi\|^2_{\mathcal{H}}$$

Hence, $\|(A-\mu)^{-1})\|_{\mathcal{L}(\mathcal{H})} = (\lambda-\mu)^{-1}$ so that Proposition 2.7 implies the claim. □

The crucial assumption of Proposition 2.8 is that the semigroup

$$\left\{e^{-tA} : t \in [0,\infty)\right\} \subset \mathcal{L}(\mathcal{H})$$

is positivity improving. The basic example of such a family is given by the one induced by the Schrödinger operator of non-interacting particles.

Example 2.21. *Consider $-\Delta : H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$. Then $\{e^{-t(-\Delta)} : t \in [0,\infty)\} \subset \mathcal{L}(\mathcal{H})$ is a family of positivity improving operators. In fact, using that the inverse Fourier transform of a Gaussian is again a Gaussian, we find for all $\varphi \in H^2(\mathbb{R}^d)$ that*

$$e^{-t(-\Delta)}\varphi(\cdot) = \frac{1}{(4\pi t)^{d/2}} \int_{\mathbb{R}^d} e^{-|\cdot - y|^2/4t}\varphi(y)\, dy = (2\pi t)^{-d/2}(e^{-|\cdot|^2/(2t)} * \varphi)$$

Hence, $e^{-t(-\Delta)}$ acts as a convolution with a positive function and is positivity improving. Notice that $[0,\infty) \ni t \mapsto \psi_t = e^{-t(-\Delta)}\varphi$ solves the heat equation:

$$\begin{cases} \partial_t \psi_t & = \Delta\psi_t, \\ (\psi_t)_{|t=0} & = \varphi. \end{cases}$$

From the fact that a typical Hamiltonian has the form $H = -\Delta + V$ with a multiplication operator V, and the fact that the operators $\left\{e^{-t(-\Delta)} : t \in [0,\infty)\right\} \subset \mathcal{L}(\mathcal{H})$ are positivity improving, one may expect that also e^{-tH} is positivity improving under suitable assumptions on V. To show this, we use the Trotter product formula, which enables us to compute the exponential of $H = -\Delta + V$ in terms of $e^{-t(-\Delta)}$ and e^{-V}.

Theorem 2.18 (Trotter-Product Formula)**.** *Let $A : D(A) \to \mathfrak{H}, B : D(B) \to \mathfrak{H}$ be self-adjoint operators on a Hilbert space $\mathfrak{H}$. Assume that A, B are bounded from below and that $A+B$ is self-adjoint on $D = D(A) \cap D(B)$. Then it holds true that*

$$e^{-(A+B)t}\psi = \lim_{n\to\infty} (e^{-At/n}e^{-Bt/n})^n\psi$$

for every $\psi \in D$ and $t \in [0,\infty)$.

Proof. Suppose w.l.o.g. that $A, B \geq 0$, such that the norms of the operators $e^{-As} \in \mathcal{L}(\mathfrak{H})$, $e^{-Bs} \in \mathcal{L}(\mathfrak{H})$ and $e^{-(A+B)s} \in \mathcal{L}(\mathfrak{H})$ are all bounded by one, uniformly in $s \in [0,\infty)$.

For $\psi \in D$ and $t \in [0,\infty)$, we write

$$\begin{aligned} &\left[(e^{-At/n}e^{-Bt/n})^n - (e^{-(A+B)t/n})^n\right]\psi \\ &= \sum_{k=0}^{n-1} \left[e^{-At/n}e^{-Bt/n}\right]^k \left[e^{-At/n}e^{-Bt/n} - e^{-(A+B)t/n}\right] \left[e^{-(A+B)t/n}\right]^{n-1-k}\psi. \end{aligned} \tag{2.23}$$

Note that e^{-As}, e^{-Bs} and $e^{-(A+B)s}$, leave D invariant (e.g. by the spectral theorem), for every $s \in [0,\infty)$. We thus conclude that

$$\begin{aligned} &\big\| \big[(e^{-At/n} e^{-Bt/n})^n - (e^{-(A+B)t/n})^n \big] \psi \big\|_{\mathfrak{H}} \\ &\leq |t| \sup_{s\in[0,t]} \big\| (t/n)^{-1} \big[e^{-At/n} e^{-Bt/n} - e^{-(A+B)t/n} \big] e^{-(A+B)s} \psi \big\|_{\mathfrak{H}} \end{aligned} \tag{2.24}$$

Now, for every $\varphi \in D = D(A) \cap D(B) = D(A+B)$, we have that

$$\begin{aligned} & t^{-1}(e^{-At} e^{-Bt} - e^{-(A+B)t})\varphi \\ &= \Big(\frac{1}{t}(e^{-tA} - 1)\varphi + (e^{-tA} - 1)\frac{1}{t}(e^{-Bt} - 1)\varphi - \frac{1}{t}(e^{-(A+B)t} - 1)\varphi \Big) \\ &= \int_0^1 dx\, e^{-Atx} A\varphi + (e^{-tA} - 1) \int_0^1 dx\, e^{-Btx} B\varphi - \int_0^1 dx\, e^{-(A+B)tx}(A+B)\varphi. \end{aligned}$$

This implies for every $\varphi, \psi \in D$ and every $s \in [0,\infty)$ that

$$\lim_{t\to 0} t^{-1} \big[e^{-At} e^{-Bt} - e^{-(A+B)t} \big] e^{-(A+B)s} \psi = 0.$$

On the other hand, an application of the uniform boundedness principle implies that

$$\sup_{t\geq 0} \| t^{-1}(e^{-At} e^{-Bt} - e^{-(A+B)t})\psi \| \leq C \|\psi\|_D$$

for $\|\psi\|_D = \|\psi\|_{\mathfrak{H}} + \|(A+B)\psi\|_{\mathfrak{H}}$. For fixed $t \geq 0$ and $\psi \in D$, $\big\{ e^{-(A+B)s}\psi : s \in [0,t] \big\} \subset D$ is compact in D equipped with $\|\psi\|_D$ (recall that D then becomes a Banach space by closedness of $A+B$): it is the image of the compact set $[0,t]$ under the continuous map $\mathbb{R} \ni \tau \mapsto e^{-(A+B)\tau}\psi \in (D, \|\cdot\|_D)$. Combining a simple covering argument with the two previous observations thus implies the uniform convergence

$$\lim_{t\to 0} \sup_{s\in[0,t]} \big\| (t/n)^{-1} \big[e^{-At/n} e^{-Bt/n} - e^{-(A+B)t/n} \big] e^{-(A+B)s} \psi \big\|_{\mathfrak{H}} = 0.$$

□

The next corollary shows that trapping Hamiltonians have unique ground states.

Corollary 2.7. *Let $H = -\Delta + V : D(H) \to L^2(\mathbb{R}^d)$ be self-adjoint, let $V \in L^\infty_{loc}(\mathbb{R}^d)$ bounded from below and assume that $C_c^\infty(\mathbb{R}^d)$ is a core for H. Suppose, moreover, that $\lambda = \inf \sigma(H) \in \mathbb{R}$ is an eigenvalue of H. Then, $\inf \sigma(H)$ is a simple eigenvalue and the corresponding eigenvector is positive after multiplication by a constant phase.*

Proof. Assume w.l.o.g. $V \geq 0$. By Proposition 2.8, the claim follows if

$$\big\{ e^{-Ht} : t \in [0,\infty) \big\} \subset \mathcal{L}(\mathcal{H})$$

is a family of positivity improving maps. To apply the Trotter-Product Formula 2.18, we first approximate H by $H_n = -\Delta + V_n$ where $V_n = V\chi\big(V^{-1}([0,n])\big) \in L^\infty(\mathbb{R}^d)$.

Then $H_n : H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is self-adjoint and essentially self-adjoint on $C_c^\infty(\mathbb{R}^d)$ for all $n \in \mathbb{N}$ by Theorem 2.4. Moreover, the Trotte product formula 2.18 and Example 2.21 imply that $e^{-H_n t}$ is positivity improving for every $n \in \mathbb{N}$ and $t \in [0;\infty)$. Indeed, for $\psi \in H^2(\mathbb{R}^d)$ such that $\psi \geq 0$, $\psi \not\equiv 0$, we have that

$$\big((e^{-(-\Delta)t/m}e^{-V_n t/m})^m\psi\big)(x) \geq e^{-nt}\big(e^{-(-\Delta)t}\psi\big)(x) > 0 \quad \text{(for } a.e.\ x \in \mathbb{R}^d\text{)},$$

uniformly in $m \in \mathbb{N}$, which follows from Example 2.21 and the fact that $|V_n| \leq n$.

We would like to use this to show that $e^{-Ht} \in \mathcal{L}(\mathcal{H})$ is positivity improving, too. To this end, let's first show that $e^{-H_n t}$ converges strongly to e^{-Ht}. Applying the monotone convergence theorem, we find $\lim_{n\to\infty} \|(H - H_n)\psi\|_{\mathcal{H}} = 0$ for any $\psi \in C_c^\infty(\mathbb{R}^d)$. Thus

$$0 \leq \lim_{n\to\infty} \|(H-z)^{-1}\psi - (H_n - z)^{-1}\psi\|_{\mathcal{H}} \leq |\operatorname{Im} z|^{-1} \lim_{n\to\infty} \|(H - H_n)(H-z)^{-1}\psi\|_{\mathcal{H}} = 0$$

for any $z \in \mathbb{C}$ with $\operatorname{Im} z \neq 0$ and any $\psi \in (H - z)(C_c^\infty(\mathbb{R}^d))$. Here, we used that $\|(H_n - z)^{-1}\|_{\mathcal{L}(\mathcal{H})} \leq |\operatorname{Im} z|^{-1}$, uniformly in $n \in \mathbb{N}$. Notice also that $(H - z)(C_c^\infty(\mathbb{R}^d)) \subset \mathcal{H}$ is dense (for $\operatorname{Im}(z) \neq 0$), because $C_c^\infty(\mathbb{R}^d)$ is a core for H. As a consequence

$$\lim_{n\to\infty} \|(H-z)^{-1}\psi - (H_n - z)^{-1}\psi\|_{\mathcal{H}} = 0$$

for all $\psi \in \mathcal{H}$. From the strong convergence of the resolvents, we obtain the strong convergence of the operator exponentials as follows: recall that the Stone-Weierstrass theorem 2.24 implies that the C^*-subalgebra of $C_\infty(\mathbb{R}) = \{f \in C(\mathbb{R}) : \lim_{|x|\to\infty} f(x) = 0\}$ that is generated by $x \mapsto (x-i)^{-1}$ and $x \mapsto (x+i)^{-1}$ is dense in $C_\infty(\mathbb{R})$, equipped with the sup-norm. Indeed, we observed already in the chapter about the spectral theorem that this subalgebra separates points and is closed under conjugation in

$$\{f \in C(X) : f(\pm\infty) = 0\} \simeq C_\infty(\mathbb{R}),$$

where $X = \mathbb{R} \cup \{\pm\infty\} = \overline{\mathbb{R}}$ denotes the extended reals (as a compactification of $\mathbb{R}$).

Now, we know that $H_n \geq V_n \geq 0$ by assumption on V and that $H \geq 0$. A basic application of the spectral theorem thus implies that

$$e^{-Ht} = f(H)e^{-Ht} \qquad \text{and} \qquad e^{-H_n t} = f(H_n + n)e^{-H_n t}$$

for every $f \in C(\mathbb{R})$ which is such that $f_{|[0,\infty)} = 1$ and $f_{|(-\infty;-1)} = 0$. Since the map $\mathbb{R} \ni x \mapsto f(x)e^{-xt} \in C_\infty(\mathbb{R})$, we can thus approximate e^{-Ht} and $e^{-H_n t}$ strongly by polynomials in $(H-i)^{-1}$, $(H+i)^{-1}$ and $(H_n - i)^{-1}$, $(H_n + i)^{-1}$, respectively, so that

$$\lim_{n\to\infty} \|e^{-Ht}\psi - e^{-H_n t}\psi\|_{\mathcal{H}} = 0 \tag{2.25}$$

for every $\psi \in \mathcal{H}$ and $t \in [0,\infty)$. Since zero can not be an eigenvalue of e^{-Ht} (*exercise*), this shows that e^{-Ht} is positivity preserving for every $t \in [0,\infty)$.

What remains is to show is the stronger statement that e^{-Ht} is in fact positivity improving. Here, we argue as follows. Let $\psi \geq 0$, $\psi \not\equiv 0$, and suppose $\varphi \geq 0$ is such that $\langle \varphi, e^{-Ht}\psi\rangle = 0$ for all $t \geq 0$. Then, as a function in $L^2(\mathbb{R}^d)$, we have that

$$\varphi\, e^{-Ht}\psi = 0 \in L^2(\mathbb{R}^d).$$

Hence, also $(e^{V_n t}\varphi)\, e^{-Ht}\psi = 0$ for all $n \in \mathbb{N}$ and all $t \geq 0$. Invoking the Trotter-Product Formula, Theorem 2.18, again, we deduce that

$$\langle e^{-(H-V_n)t}\varphi, e^{-Ht}\psi\rangle_{\mathcal{H}} = \lim_{k\to\infty} \big\langle \big(e^{-Ht/k}e^{V_n t/k}\big)^k\varphi, e^{-Ht}\psi\big\rangle_{\mathcal{H}} = 0$$

and, arguing as in the previous step (*exercise*), this implies that

$$\langle e^{\Delta t}\varphi, e^{-Ht}\psi\rangle_{\mathcal{H}} = 0$$

for every $t \geq 0$. If $\varphi \not\equiv 0$, then $e^{\Delta t}\varphi(x) > 0$ for *a.e.* $x \in \mathbb{R}^d$, so $\langle e^{\Delta t}\varphi, e^{-Ht}\psi\rangle_{\mathcal{H}} > 0$ (e^{-Ht} is positivity preserving). Hence, we must have $\varphi = 0$.

In conclusion, we have proved for $\psi \geq 0, \psi \not\equiv 0$ that

$$\varphi \geq 0 \,\wedge\, \langle \varphi, e^{-Ht}\psi\rangle = 0\; \forall\, t \geq 0 \implies \varphi = 0.$$

Choosing $\varphi = \chi_{\{x\in\mathbb{R}^d:\, e^{-Ht}\psi(x)\leq 0\}}$ $(= \chi_{\{x\in\mathbb{R}^d:\, e^{-Ht}\psi(x)=0\}}$ a.s.), we get $e^{-Ht}\psi > 0$. □

We conclude this section with an interesting corollary, which is related to the path integral formulation of quantum mechanics - the Feynman-Kac formula. Our short discussion of this result is a digression and we refer to [56, Chapter X.II] and [8] for further details. Let us denote by μ_x the Wiener measure for one-dimensional Brownian motion starting at $x \in \mathbb{R}$. Wiener measure μ_x is a Gaussian probability measure and can be defined on the space $\Omega = C([0;T];\mathbb{R}) \cap \{f \in C([0;T];\mathbb{R}) : f(0) = x\}$ of continuous functions[7] starting at $x \in \mathbb{R}$. As a Gaussian measure, it is characterized by its mean $\int_\Omega d\mu_x\, \omega(t) = x$ and its covariance, which is equal to

$$C(s,t) = \int_\Omega d\mu_x(\omega)(\omega(t) - x)(\omega(s) - x) = \min(s,t).$$

In other words, the random variables $\Omega \ni \omega \mapsto \omega(t) \in \mathbb{R}$, defined on the probability space $(\Omega, \mathcal{B}(\Omega), \mu_x)$, are Gaussian with mean x and variance t. Moreover, given times $0 \leq t_0 < t_1 < \cdots < t_n$, the increments $\omega(t_1) - \omega(t_0)$, $\omega(t_2) - \omega(t_1), \ldots, \omega(t_n) - \omega(t_{n-1})$ are independent. The stochastic process $(\omega(t))_{t\in[0;T]}$ is called Brownian motion.

Referring for the more technical aspects to basic courses on stochastic processes, the measure μ_x can be constructed essentially as follows. Pick an orthonormal basis $(\varphi_k)_{k\in\mathbb{N}}$ of $L^2([0;T])$ and a sequence of independent standard Gaussian random variables $(X_k)_{k\in\mathbb{N}}$, defined on some probability space $(\Omega, \mathcal{F}, \mathbb{P})$. For $f \in L^2([0;T])$ such that

$$f = \sum_{k\in\mathbb{N}} \alpha_k \varphi_k \quad \text{with} \quad \sum_{k\in\mathbb{N}} |\alpha_k|^2 = \|f\|_2^2,$$

the random variable

$$G(f) = \sum_{k\in\mathbb{N}} \alpha_k \varphi_k$$

[7]This means that the push-forward measure $\ell_*(\mu_x)$ is a Gaussian measure on $\mathbb{R}$, for any $\ell \in \Omega^*$. Notice, for instance, that the Dirac-δ centered at $t \in [0;T]$ lies in $\delta_t \in \Omega^*$ for any $t \in [0;T]$.

is a centered Gaussian random variable with variance

$$\mathbb{E}\, G(f)^2 = \|f\|_2^2.$$

Now, define $(B_t)_{t\in[0;T]}$ by $B_t = x + G(\chi_{[0;t]})$, then it is straightforward to check that

- $B_0 = x$ $\mathbb{P}$ *a.s.*,
- finite linear combinations of the $(B_t - x)$ are centered Gaussian random variables,
- $\mathbb{E}(B_t - x)(B_s - x) = \min(s,t)$ for all $s, t \in [0;T]$.

One says the stochastic process $(B_t)_{t\in[0;T]}$ defines a Gaussian process (the map G is an isometry from L^2 to a Gaussian space) and it is called pre-Brownian motion. It satisfies all properties of Brownian motion mentioned earlier, except that the sample paths

$$[0;T] \ni t \mapsto B_t(\lambda) \in \mathbb{R}$$

need not be continuous for $\mathbb{P}$-*a.e.* $\lambda \in \Omega$. With regards to the remaining properties, notice for example that for $s \le t < u$, one has

$$\mathbb{E}(B_u - B_t)B_s = \min(u,s) - \min(t,s) = 0,$$

which implies that $B_u - B_t$ is independent of $\sigma(B_s : s \le t)$ by basic properties of Gaussian processes. In courses on stochastic processes, one then learns how to modify $(B_t)_{t\in[0;T]}$ to another process $(\omega(t))_{t\in[0;T]}$ such that

$$t \mapsto \omega_t(\lambda) \text{ is continuous for every } \lambda \in \Omega \text{ and } \mathbb{P}(\{B_t = \omega_t\}) = 1\,\forall t \in [0;T].$$

Wiener measure μ_x is then defined as the law (the push-forward measure) of the random variable $(\Omega, \mathcal{F}, \mathbb{P}) \in \omega \mapsto \big([0;T] \ni t \mapsto \omega_t \in C([0;T];\mathbb{R})\big)$. For a detailed introductory discussion of Brownian motion and their properties, see for example [33].

Assuming the existence of μ_x and $(\omega(t))_{t\in[0;T]}$ as above, we see that

$$\int_\Omega d\mu_x(\omega) f(\omega(t)) = \int_{\mathbb{R}} \frac{e^{-(y-x)^2/2t}}{\sqrt{2\pi t}} f(y)\, dy$$

for every $f \in L^2(\mathbb{R})$. At the same time, we recognize that for *a.e.* $x \in \mathbb{R}$, we have that

$$\int_{\mathbb{R}} \frac{e^{-(y-x)^2/2t}}{\sqrt{2\pi t}} f(y)\, dy = \big(e^{-t(-\Delta/2)} f\big)(x),$$

which relates Brownian motion to the free heat semigroup $\big\{e^{-t(-\Delta/2)} : t \ge 0\big\}$. The Feynman-Kac formula tells us similarly how to compute $\big(e^{-t(-\Delta/2+V)} f\big)(x)$ for suitable potentials V in terms of a path integral over the Wiener measure.

Corollary 2.8 (Feynman-Kac Formula)**.** *Let $V \in C_c(\mathbb{R})$, then for all $f \in L^2(\mathbb{R})$*

$$\big(e^{-t(-\Delta/2+V)} f\big)(x) = \int_\Omega d\mu_x(\omega) f(\omega(t)) \exp\bigg(- \int_0^t V(\omega(s))\, ds\bigg).$$

Proof. The proof follows from the Trotter-product formula (it is left as an *exercise* to check that we may apply the formula). Indeed, we claim that

$$\begin{aligned}\Big(\big(e^{-(-\Delta/2)t/n}e^{-Vt/n}\big)^n f\Big)(x) &= \int_{\mathbb{R}}\int_{\mathbb{R}}\cdots\int_{\mathbb{R}} p(x;x_n;t/n)p(x_n;x_{n-1};t/n)\dots p(x_2;x_1;t/n)\\ &\qquad\times \exp\Big(-\frac{t}{n}\sum_{j=1}^{n} V(x_j)\Big) f(x_1)\,dx_1dx_2\dots dx_n\\ &= \int_{\Omega} \exp\Big(-\frac{t}{n}\sum_{j=1}^{n} V(\omega(jt/n))\Big) f(\omega(t))\,d\mu_x(\omega),\end{aligned} \tag{2.26}$$

where p denotes the heat kernel, i.e.

$$p(x;y;t) = \frac{e^{-(x-y)^2/2t}}{\sqrt{2\pi t}}\ \big(= p(x-y;0;t) = p(0;x-y;t)\big).$$

While the first equality follows simply by iteration (*exercise*), for the second equality we use the fact that $\big(\omega((j+1)t/n)-\omega(jt/n)\big)_{j=1}^{n-1}$ are i.i.d. Gaussian under μ_x with the increment $\omega((j+1)t/n)-\omega(jt/n)$ having variance t/n for all $j=1,\dots,n$. Indeed, let's verify the second step for $n=2$ and leave the general case as an *exercise*. We compute

$$\begin{aligned}&\int_{\Omega}\exp\Big(-\frac{t}{2}V(\omega(t/2))-\frac{t}{2}V(\omega(t))\Big)f(\omega(t))\,d\mu_x(\omega)\\ &= \int_{\Omega}\exp\Big(-\frac{t}{2}V(\omega(t/2))-\frac{t}{2}V\big((\omega(t)-\omega(t/2))+\omega(t/2)\big)\Big)f(\omega(t))\,d\mu_x(\omega)\\ &= \int_{\mathbb{R}}\int_{\mathbb{R}} p(y_1;x;t/2)p(y_2;0;t/2)\exp\Big(-\frac{t}{2}V(y_1)-\frac{t}{2}V(y_2+y_1)\Big)f(y_2+y_1)\,dy_1dy_2\\ &= \int_{\mathbb{R}}\int_{\mathbb{R}} p(x;x_2;t/2)p(x_1;x_2;t)\exp\Big(-\frac{t}{2}V(x_1)-\frac{t}{2}V(x_2)\Big)f(x_1)\,dx_1dx_2.\end{aligned}$$

Generalizing the above computation to arbitrary $n\in\mathbb{N}$, we conclude (2.26). Finally, taking the limit $n\to\infty$ for a suitable subsequence on the l.h.s. by the Trotter formula (to obtain the *a.e.* equality in $L^2(\mathbb{R})$) and applying the dominated convergence theorem on the r.h.s., using that $V\in C_c(\mathbb{R})$ as well as

$$\lim_{n\to\infty}\frac{t}{n}\sum_{j=1}^{n}V(\omega(jt/n)) = \int_0^t V(\omega(s))\,ds$$

for each path $\omega\in\Omega$, we conclude the theorem. □

Remark. *The Feynman-Kac formula is also valid in higher dimensions and with much weaker assumptions on the potential, see e.g. [56, Theorem X.68]. For the sake of simplicity, in Corollary 2.8, we focus on dimension one and potentials $V\in C_c(\mathbb{R})$. For interesting applications of the Feynman-Kac formula, see for instance [64].*

2.5.4 Quadratic Forms and Self-Adjoint Operators

In this section, we discuss basic results about quadratic forms. We show that every closed, semibounded form corresponds to a unique self-adjoint operator. As a basic application, we introduce the Laplacian with Dirichlet and Neumann boundary conditions.

Given a dense linear space of a Hilbert space $\mathcal{H}$, we call a map $q : Q(q) \times Q(q) \to \mathbb{C}$ a quadratic form with form domain $Q(q)$ if $\varphi \mapsto q(\varphi, \psi)$ is anti-linear and $\psi \mapsto q(\varphi, \psi)$ is linear, for every $\psi, \varphi \in Q(q)$. We say that q is non-negative if $q(\psi, \psi) \geq 0$ for all $\psi \in Q(q)$ and, more generally, we call q semibounded if $q(\psi, \psi) \geq c\|\psi\|_{\mathcal{H}}^2$ for some $c \in \mathbb{R}$. Finally, we say that q is symmetric if $q(\psi, \varphi) = \overline{q(\varphi, \psi)}$ for all $\varphi, \psi \in Q(q)$.

In the setting of complex Hilbert spaces $\mathcal{H}$, notice that a form is symmetric if it is semibounded. Indeed, semiboundedness implies that $q(\zeta, \zeta) \in \mathbb{R}$ so that by polarization

$$\begin{aligned} 4\,q(\varphi, \psi) &= q(\varphi + \psi, \varphi + \psi) - q(\varphi - \psi, \varphi - \psi) - iq(\varphi + i\psi, \varphi + i\psi) + iq(\varphi - i\psi, \varphi - i\psi) \\ &= q(\psi + \varphi, \psi + \varphi) - q(\psi - \varphi, \psi - \varphi) - iq(\psi - i\varphi, \psi - i\varphi) + iq(\psi + i\varphi, \psi + i\varphi) \\ &= 4\,\overline{q(\psi, \varphi)}. \end{aligned}$$

We call a semibounded quadratic form $q : Q(q) \times Q(q) \to \mathbb{C}$ s.t. $q(\varphi, \varphi) \geq -M\|\varphi\|_{\mathcal{H}}^2$ closed if the form domain $Q(q)$ is a Hilbert space when equipped with

$$\langle \psi, \varphi \rangle_{+1} = q(\psi, \varphi) + (M + 1)\langle \psi, \varphi \rangle_{\mathcal{H}}.$$

If q is closed and $D \subset Q(q)$ is dense with respect to the induced norm $\| \cdot \|_{+1}$, we call D a form core for q. We say that q is closable if it has a closed extension. If q is closable and has a smallest closed extension, we call the latter its closure.

Lemma 2.10. *Let $q : Q(q) \times Q(q) \to \mathbb{C}$ be a semibounded quadratic form. Then q is closed if and only if whenever $(\psi_n)_{n\in\mathbb{N}}$ is a sequence in $Q(q)$ that converges to ψ in $\mathcal{H}$ and is such that $q(\psi_n - \psi_m, \psi_n - \psi_m) \to 0$ as $n, m \to \infty$, then $\psi \in Q(q)$ and $\lim_{n\to\infty} q(\psi_n - \psi, \psi_n - \psi) = 0$.*

Proof. Suppose that q is closed and suppose $(\psi_n)_{n\in\mathbb{N}}$ in $Q(q)$ converges to ψ in $\mathcal{H}$ and is such that $q(\psi_n - \psi_m, \psi_n - \psi_m) \to 0$ as $n, m \to \infty$. This clearly implies that $(\psi_n)_{n\in\mathbb{N}}$ is Cauchy with respect to the induced norm $\| \cdot \|_{+1}$. By completeness, $(\psi_n)_{n\in\mathbb{N}}$ has a limit in $\mathcal{H}_{+1} = \big(Q(q), \langle \cdot, \cdot \rangle_{+1}\big)$, call it φ. Since $\|\psi_n - \varphi\|_{\mathcal{H}} \leq \|\psi_n - \varphi\|_{+1} \to 0$ as $n \to \infty$, we conclude that $\varphi = \psi \in Q(q)$ and hence $\lim_{n\to\infty} q(\psi_n - \psi, \psi_n - \psi) = 0$.

On the other hand, suppose q is a form with the property that whenever $(\psi_n)_{n\in\mathbb{N}}$ is a sequence in $Q(q)$ that converges to ψ in $\mathcal{H}$ and is such that $q(\psi_n - \psi_m, \psi_n - \psi_m) \to 0$ as $n, m \to \infty$, then $\psi \in Q(q)$ and $\lim_{n\to\infty} q(\psi_n - \psi, \psi_n - \psi) \to 0$. Then suppose that $(\varphi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathcal{H}_{+1}$. Again, by $\| \cdot \|_{\mathcal{H}} \leq \| \cdot \|_{+1}$, we find that $(\varphi_n)_{n\in\mathbb{N}}$ has a limit φ in $\mathcal{H}$ and, moreover, $q(\varphi_n - \varphi_m, \varphi_n - \varphi_m) \to 0$. Thus, $\varphi \in Q(q)$ and $\lim_{n\to\infty} \varphi_n = \varphi$ in $\mathcal{H}_{+1}$, so q is closed. □

Example 2.22. *Suppose that $A : D(A) \to \mathcal{H}$ is a self-adjoint operator. By the spectral theorem, suppose w.l.o.g. that $\mathcal{H} = L^2(\Omega, \mathcal{B}(\Omega), \mu)$ and that $A = A_f$ corresponds to* *multiplication by $f : \Omega \to \mathbb{R}$ on $D(A) = \{\psi \in L^2(d\mu) : f\,\psi \in L^2(d\mu)\}$. Define*

$$Q(A) = \Big\{\psi \in L^2(d\mu) : \int_\Omega d\mu(x)|f(x)||\psi(x)|^2 < \infty\Big\} \,\big(= D(|A|^{1/2})\big)$$

and $q : Q(A) \times Q(A) \to \mathbb{C}$ by

$$q(\psi, \varphi) = \int_\Omega d\mu(x) f(x)\,\overline{\psi}(x)\varphi(x).$$

Then q is called the quadratic form associated to A and $Q(A)$ is called the form domain of the operator A. By slight abuse of notation, we sometimes write $q(\psi, \varphi) = \langle \psi, A\varphi\rangle_{\mathcal{H}}$ although $A\varphi$ need not make sense for all $\varphi \in Q(A)$.

Suppose A is semibounded such that q is a semibounded form. Then q is closed. Indeed, assume w.l.o.g. that $A \geq 0$ so that $f(x) \geq 0$ for μ-a.e. $x \in \Omega$. Let $(\psi_n)_{n\in\mathbb{N}}$ be a sequence in $Q(A)$ that converges to ψ in $\mathcal{H}$ and that is such that

$$\int_\Omega d\mu(x) f(x)|(\psi_n - \psi_m)(x)|^2 \to 0 \quad as \quad n, m \to \infty.$$

By completeness of $L^2(\mu)$, we see that $(f^{1/2}\psi_n)_{n\to\infty}$ converges in $L^2(\mu)$ to some $\varphi \in L^2(d\mu)$. Choosing suitable pointwise almost surely converging subsequences, we must have that $\varphi = f^{1/2}\psi$ μ a.s. so that $f^{1/2}\psi \in L^2(d\mu)$, i.e. $\psi \in Q(A)$, and

$$\int_\Omega d\mu(x) f(x)|(\psi_n - \psi)(x)|^2 \to 0 \quad as \quad n \to \infty.$$

Problem 2.23. *Let $q : Q(A) \times Q(A) \to \mathbb{C}$ be the form w.r.t. a semibounded self-adjoint operator $A : D(A) \to \mathcal{H}$. Prove that any operator core of A is a form core for q.*

Our first main result about quadratic forms is the following.

Theorem 2.19. *Let $q : Q(q) \times Q(q) \to \mathbb{C}$ be a semibounded, closed quadratic form. Then, there exists a unique self-adjoint operator $A : D(A) \to \mathcal{H}$ such that q is the quadratic form associated to A, that is, $q(\psi, \varphi) = \langle \psi, A\varphi\rangle_{\mathcal{H}}$ as in Example 2.22.*

Proof. We assume without loss of generality that q is non-negative. As above, we denote by $\mathcal{H}_{+1}$ the Hilbert space $(Q(q), \langle\cdot,\cdot\rangle_{+1})$. We then denote by $\mathcal{H}_{-1}$ the space of bounded *conjugate linear* functionals on $\mathcal{H}_{+1}$. Analogously to the usual Riesz representation theorem, every $\ell \in \mathcal{H}_{-1}$ is uniquely represented by some $\psi_\ell \in \mathcal{H}_{+1}$. More precisely, the canonical linear isomorphism that sends $\psi \in \mathcal{H}_{+1}$ to $\Phi(\psi) \in \mathcal{H}_{-1}$, defined by

$$\Phi(\psi)(\varphi) = \langle \varphi, \psi\rangle_{+1} = q(\varphi, \psi) + \langle \varphi, \psi\rangle_{\mathcal{H}},$$

is an isometric isomorphism of $\mathcal{H}_{+1}$ into $\mathcal{H}_{-1}$. Finally, we denote by $i : \mathcal{H}_{+1} \to \mathcal{H}$ the canonical embedding of $\mathcal{H}_{+1}$ into $\mathcal{H}$ and by $j : \mathcal{H} \to \mathcal{H}_{-1}$ the embedding of $\mathcal{H}$ into $\mathcal{H}_{-1}$ that is defined by $j(\psi) = \langle\cdot, \psi\rangle_{\mathcal{H}}$. Notice that

$$|j(\psi)(\varphi)| \leq \|\psi\|_{\mathcal{H}}\|\varphi\|_{\mathcal{H}} \leq \|\psi\|_{\mathcal{H}}\|\varphi\|_{+1}$$

so that $j(\psi) \in \mathcal{H}_{-1}$ with $\|j(\psi)\|_{\mathcal{H}_{-1}} \leq \|\psi\|_{\mathcal{H}}$. With i and j as above, we have that

$$\mathcal{H}_{+1} \stackrel{i}{\hookrightarrow} \mathcal{H} \stackrel{j}{\hookrightarrow} \mathcal{H}_{-1}.$$

To prove the theorem, we find a self-adjoint operator $B : D(B) \to \mathcal{H}$ such that

$$\langle \varphi, B\psi \rangle_{\mathcal{H}} = q(\varphi, \psi) + \langle \varphi, \psi \rangle_{\mathcal{H}} = \langle \varphi, \psi \rangle_{\mathcal{H}_{+1}} = \Phi(\psi)(\varphi) \tag{2.27}$$

for a suitable dense domain $D(B)$. Once we find such an operator, it will be simple to conclude that the quadratic form q is the form associated to $A = B - \mathbf{1}_{\mathcal{H}}$.

To find the right operator B, eq. (2.27) motivates to define

$$\begin{aligned} D(B) =& \{\psi \in \mathcal{H}_{+1} \subset \mathcal{H} : \Phi(\psi) \in \operatorname{Ran}(j)\} = \Phi^{-1}\big(\operatorname{Ran}(j)\big), \\ B =& (j^{-1})_{|\operatorname{Ran}(j)} \Phi : D(B) \to \mathcal{H}, \end{aligned}$$

Indeed, this implies for $\psi \in D(B)$ that

$$\langle \varphi, B\psi \rangle_{\mathcal{H}} = j(B\psi)(\varphi) = \Phi(\psi)(\varphi).$$

B is certainly a symmetric operator, because for all $\psi, \varphi \in D(B)$, we have

$$\langle \varphi, B\psi \rangle_{\mathcal{H}} = \Phi(\psi)(\varphi) = q(\varphi, \psi) + \langle \varphi, \psi \rangle_{\mathcal{H}} = \overline{q(\psi, \varphi) + \langle \psi, \varphi \rangle_{\mathcal{H}}} = \langle B\varphi, \psi \rangle_{\mathcal{H}}.$$

Let us show next that $D(B) \subset \mathcal{H}$ is dense. To this end, we first argue that $\operatorname{Ran}(j)$ is dense in $\mathcal{H}_{-1}$. For if not, we find some $0 \neq \zeta \in \mathcal{H}_{-1}^*$ that vanishes on $\operatorname{Ran}(j)$. By duality (more precisely, using that $\mathcal{H}_{+1}$ is isometrically isomorphic to $\mathcal{H}_{-1}^*$), ζ corresponds to some $0 \neq \varphi_\zeta \in \mathcal{H}_{+1} \subset \mathcal{H}$ so that in particular

$$\zeta(j(\psi)) = j(\psi)(\varphi_\zeta)$$

for all $\psi \in \mathcal{H}$. This means that $0 = j(\psi)(\varphi_\zeta) = \langle \varphi_\zeta, \psi \rangle_{\mathcal{H}}$ for every $\psi \in \mathcal{H}$. But this is not possible, because $\varphi_\zeta \neq 0$. Thus, $\operatorname{Ran}(j)$ is dense in $\mathcal{H}_{-1}$ and since Φ is an isometric isomorphism, $D(B) = \Phi^{-1}(\operatorname{Ran}(j))$ is dense in $\mathcal{H}_{+1}$. Since, moreover, $\|\cdot\| \leq \|\cdot\|_{+1}$, we conclude that $D(B)$ is dense in $\mathcal{H}$.

Finally, we argue that B is self-adjoint. To this end, consider the linear operator $C : \Phi^{-1}j : \mathcal{H} \to \mathcal{H}_{+1} \subset \mathcal{H}$: it is clearly injective and it is symmetric, because its inverse B is symmetric. Since it is defined on all of $\mathcal{H}$, it is self-adjoint. By the spectral theorem, its inverse $B = C^{-1} : \operatorname{ran}(C) \to \mathcal{H}$ is self-adjoint as well (*exercise*).

Finally, to conclude that A is the unique self-adjoint operator whose form corresponds to q, suppose that q is also the form associated to a self-adjoint operator $\widetilde{A} : D(\widetilde{A}) \to \mathcal{H}$ and suppose w.l.o.g. that $A, \widetilde{A} \geq 1$ so that $0 \in \rho(A) \cap \rho(\widetilde{A})$. Then, $Q(A) = D(A^{1/2})$, $Q(\widetilde{A}) = D(\widetilde{A}^{1/2})$ (viewing both $A^{1/2}, \widetilde{A}^{1/2}$ as self-adjoint operators in their canonical form) and in particular $A^{-1/2}\psi \in Q(A) = Q(\widetilde{A}) = Q(q)$ for every $\psi \in \mathcal{H}$. But then

$$\begin{aligned} \langle \psi, \varphi \rangle_{\mathcal{H}} = \langle A^{1/2}A^{-1/2}\psi, A^{1/2}A^{-1/2}\varphi \rangle_{\mathcal{H}} &= q(A^{-1/2}\psi, A^{-1/2}\varphi) \\ &= \langle \widetilde{A}^{1/2}A^{-1/2}\psi, \widetilde{A}^{1/2}A^{-1/2}\varphi \rangle_{\mathcal{H}} \end{aligned}$$

for all $\psi, \varphi \in \mathcal{H}$, which implies that $U = \widetilde{A}^{1/2}A^{-1/2}$ is unitary. This means that $UU^* = \mathbf{1}_{\mathcal{H}} = \widetilde{A}^{1/2}A^{-1}\widetilde{A}^{1/2}$ s.t. $\widetilde{A}^{-1} = A^{-1}$ and therefore $D(A) = D(\widetilde{A})$ and $A = \widetilde{A}$. □

Example 2.23. *In* $L^2(\mathbb{R})$*, set* $Q(q) = C_c^\infty(\mathbb{R})$ *and define* $q : Q(q) \times Q(q) \to \mathbb{C}$ *through*

$$q(f, g) = \overline{f}(0)g(0).$$

Clearly, q *is a non-negative quadratic form. Does it correspond to a self-adjoint operator? We might suspect that this is not the case, because otherwise* q *would correspond to multiplication by a Dirac* δ*-function. In fact,* q *does not correspond to a self-adjoint operator, otherwise it would be closed. But choosing a sequence of functions* $(\varphi_n)_{n\in\mathbb{N}}$ *in* $Q(q)$ *such that* $0 \le \varphi_n \le 1$ *with supp*$(\varphi_n) \subset B_{1/n}(0)$ *and such that* $(\varphi_n)_{|B_{1/4n}(0)} = 1$ *while* $(\varphi_n)_{|\mathbb{R}\setminus B_{1/2n}(0)} = 0$*, we see that* $\lim_{n\to\infty} \varphi_n = 0$ *in* $L^2(\mathbb{R})$ *as well as* $\lim_{m,n\to\infty} q(\varphi_n - \varphi_m, \varphi_n - \varphi_m) = 0$*, but* $q(\varphi_n, \varphi_n) = 1 \neq q(0, 0)$*. Hence,* q *is not closed. The argument also shows that* q *does not have a closed extension with form core* $C_c^\infty(\mathbb{R})$*.*

Our second main result with regards to quadratic forms introduces the Friedrich's extension. In general, one might start out with a semibounded, symmetric operator $A : D(A) \to \mathcal{H}$ and it is a priori not clear how many self-adjoint extensions the operator has and which one to pick. The Friedrich's extension is a particular self-adjoint extension with a number of desirable properties, most importantly that the domain of the original *symmetric* operator is a form core for the form associated to the Friedrich's extension. This implies, for instance, that the ground state energy of the extension can already be computed (via Theorem 2.17) based on knowing the domain $D(A)$.

Theorem 2.20 (Friedrich's Extension)**.** *Let* $A : D(A) \to \mathcal{H}$ *be a non-negative and symmetric operator. Define the quadratic form* q *on* $D(A) \times D(A)$ *through*

$$q(\psi, \varphi) = \langle \psi, A\varphi \rangle_{\mathcal{H}}.$$

Then q *is a closable quadratic form and its closure* $\widehat{q}$ *is the quadratic form of a unique self-adjoint operator* $\widehat{A} : D(\widehat{A}) \to \mathcal{H}$*, the Friedrich's extension.* $\widehat{A}$ *is a non-negative extension of* A *and* $D(A)$ *is a form core for* $\widehat{q}$*. Furthermore,* $\widehat{A}$ *is the only self-adjoint extension of* A *with its domain being a subset* $D(\widehat{A}) \subset Q(\widehat{q})$ *of the form domain of* $\widehat{q}$*.*

Proof. As before, we set $\langle \psi, \varphi \rangle_{+1} = q(\psi, \varphi) + \langle \psi, \varphi \rangle_{\mathcal{H}}$. Since A is non-negative, $\langle \cdot, \cdot \rangle_{+1}$ defines an inner product on $D(A)$ and we can consider its completion $\mathcal{H}_{+1}$. What we would like to show is that $\mathcal{H}_{+1} \hookrightarrow \mathcal{H}$ can be identified with a subset of $\mathcal{H}$. If that's the case, it follows that q is closable and we obtain its semibounded closure $\widehat{q}$ with form domain $\mathcal{H}_{+1} \subset \mathcal{H}$. Notice also that $D(A)$ is then a form core for $\widehat{q}$, by construction.

Let's denote by $i : D(A) \to \mathcal{H}$ the identity map. Since $\|\cdot\|_{\mathcal{H}} \le \|\cdot\|_{+1}$, i is bounded from the dense set $D(A) \subset \mathcal{H}_{+1}$ into $\mathcal{H}$. In particular, i has a bounded extension $\widehat{i} : \mathcal{H}_{+1} \to \mathcal{H}$. We claim that $\widehat{i}$ is injective, showing that $\mathcal{H}_{+1} \hookrightarrow \mathcal{H}$. To see that $\widehat{i}$ is injective, suppose that $\widehat{i}(\varphi) = 0$. By definition of $\widehat{i}$, this means there exists a sequence $(\varphi_n)_{n\in\mathbb{N}}$ in $D(A)$ such that $\lim_{n\to\infty} \|\varphi - \varphi_n\|_{+1} = 0$ and such that $\lim_{n\to\infty} \|i(\varphi_n)\|_{\mathcal{H}} = \lim_{n\to\infty} \|\varphi_n\|_{\mathcal{H}} = 0$. This implies that

$$\|\varphi\|_{+1}^2 = \lim_{m\to\infty} \lim_{n\to\infty} \langle \varphi_n, \varphi_m \rangle_{+1} = \lim_{m\to\infty} \lim_{n\to\infty} \big(\langle \varphi_n, A\varphi_m \rangle_{\mathcal{H}} + \langle \varphi_n, \varphi_m \rangle_{\mathcal{H}} \big) = 0,$$

hence $\varphi = 0 \in \mathcal{H}_{+1}$. Observe that the non-negativity of A is used to define $\widehat{i}$ while the fact that q is defined through A implies that $\widehat{i}$ is injective.

We conclude from the previous argument that $\mathcal{H}_{+1} \hookrightarrow \mathcal{H}$ so that q has a closure $\widehat{q}$. As a semibounded, closed form, $\widehat{q}$ corresponds to a unique self-adjoint operator $\widehat{A}$, by Theorem 2.19. More precisely, $\widehat{q}$ is the form associated to $\widehat{A}$ and $D(\widehat{A}) \subset Q(\widehat{q})$ is a form core. Moreover, $\widehat{A}$ extends A. For if $\varphi \in D(A)$ and $\psi \in D(\widehat{A}) \subset Q(\widehat{q})$, then

$$\langle A\varphi, \psi\rangle_{\mathcal{H}} = \widehat{q}(\varphi, \psi) = \langle \varphi, \widehat{A}\psi\rangle_{\mathcal{H}},$$

so that $\varphi \in D(\widehat{A}^*) = D(\widehat{A})$ with $\widehat{A}^*\varphi = \widehat{A}\varphi = A\varphi$, that is $A \subset \widehat{A}$. If $\widetilde{A}$ is any other symmetric extension of A with $D(\widetilde{A}) \subset Q(\widehat{q})$, then the same argument shows that $\widehat{A}$ extends $\widetilde{A}$; in particular, if $\widetilde{A}$ is self-adjoint, then $\widetilde{A} = \widehat{A}$. □

Example 2.24. *In $L^2(I)$ for $I = (0, 1)$, consider $A = -\partial_x^2$ on $C_c^\infty(I)$. Then*

$$\|\psi\|_{+1}^2 = \|\partial_x\psi\|_{\mathcal{H}}^2 + \|\psi\|_{\mathcal{H}}^2$$

corresponds to the $H^1(I)$-norm. In particular, if $\lim_{n\to\infty}\psi_n = \psi$ in $\mathcal{H}_{+1}$, then $\psi \in H^1(I)$ extends to an absolutely continuous function in $[0, 1]$ and we have that

$$\lim_{n\to\infty}\psi_n(x) = \psi(x)$$

for every $x \in [0, 1]$ so that $\psi(0) = \psi(1) = 0$. This means that the Friedrich's extension $\widehat{A}$ of A is the self-adjoint extension of $-\partial_x^2$ with Dirichlet boundary conditions. The spectrum of this operator is explicitly given by $\sigma(\widehat{A}) = \{(n\pi)^2 : n \in \mathbb{N}\}$ and the eigenfunctions are given by $\{x \mapsto \sin(n\pi x) \in C^\infty([0, 1]) : n \in \mathbb{N}\}$ (exercise).

Using $\widehat{A}$, this implies the so called Wirtinger's inequality

$$\int_0^1 dx\,|\varphi'(x)|^2 \geq \pi^2 \int_0^1 dx\,|\varphi(x)|^2,$$

valid for all $\varphi \in C_c^\infty((0, 1))$, which follows from the lower bound on $\widehat{A}$. Notice that this lower bound is also true for the form induced by A.

Notice here that, in general, a self-adjoint extension of A need not satisfy the same lower bound like the form induced by A. For instance, another self-adjoint extension of A is the Laplacian $-\Delta_N : D(-\Delta_N) \to L^2(\mathbb{R})$ with Neumann boundary conditions, defined by $D(-\Delta_N) = \{\varphi \in H^2([0, 1]) : \varphi'(0) = \varphi'(1) = 0\}$. In this case, the lowest eigenvalue $\lambda_1^{(N)}$ of $-\Delta_N$ corresponds to $\lambda_1^{(N)} = 0$, with constant eigenfunction.

The previous example mentions the Dirichlet and Neumann Laplacians, encountered in many PDE problems. We finish this section with their definition for general domains $\Omega \subset \mathbb{R}^n$ and with their characterization when Ω is a box. We refer to the monograph [61] for more details on self-adjoint realizations of the Laplacian on general domains.

Assume that $\Omega \subset \mathbb{R}^n$ is open. The Dirichlet Laplacian $-\Delta_D^\Omega$ is defined as the Friedrich's extension of the non-negative, symmetric operator $-\Delta : C_c^\infty(\Omega) \to L^2(\Omega, dx)$.

In other words, $-\Delta_D^\Omega$ is the unique self-adjoint operator whose form corresponds to the closure of the form

$$(\psi, \varphi) \mapsto \int_\Omega dx\, \overline{\nabla\psi}(x) \cdot \nabla\varphi(x)$$

on $C_c^\infty(\Omega)$. On the other hand, the Neumann Laplacian $-\Delta_N^\Omega$ is the unique self-adjoint operator whose assocated form is equal to

$$(\psi, \varphi) \mapsto \int_\Omega dx\, \overline{\nabla\psi}(x) \cdot \nabla\varphi(x)$$

on the domain $H^1(\Omega)$. Note in particular that this form is closed in $H^1(\Omega)$.

Proposition 2.9. *Suppose that $\Omega = (-1,1)^n \subset \mathbb{R}^n$ is a cube and denote by $-\Delta_D$ and $-\Delta_N$ the Dirchlet and, respectively, Neumann Laplacian for this domain. Then:*

a) $D_D = \{f \in C^\infty(\overline{\Omega}) : f_{|\partial\Omega} = 0\}$ is an operator core for $-\Delta_D$ and for such $f \in D_D$, we have that

$$-\Delta_D f = -\sum_{i=1}^n \partial_i^2 f.$$

b) $D_N = \{f \in C^\infty(\overline{\Omega}) : (\partial f/\partial\widehat{n})_{|\partial\Omega} = (\nabla f \cdot \widehat{n})_{|\partial\Omega} = 0\}$ is an operator core for $-\Delta_N$, where $\widehat{n}$ denotes the outward pointing unit normal to Ω. For $f \in D_N$, we have that

$$-\Delta_N f = -\sum_{i=1}^n \partial_i^2 f.$$

Proof. The proofs of $a)$ and $b)$ are similar. We focus on $b)$ and leave $a)$ as an exercise. Before we start, let us mention why D_N is a natural domain to consider: if the form

$$(f, g) \mapsto \langle \nabla f, \nabla g\rangle = \int_\Omega dx\, \overline{\nabla f}(x) \cdot \nabla g(x) = \langle f, -\Delta_N g\rangle$$

corresponds to a suitable self-adjoint operator $-\Delta_N$ that acts like the usual Laplacian on $f, g \in C^\infty(\overline{\Omega})$, then by Stokes theorem we have that

$$\langle f, -\Delta_N g\rangle = \langle \nabla f, \nabla g\rangle - \int_{\partial\Omega} d\mathcal{S}\, f \frac{\partial g}{\partial \widehat{n}}.$$

But this is only possible if $(\partial f/\partial\widehat{n})_{|\partial\Omega} = (\partial g/\partial\widehat{n})_{|\partial\Omega} = 0$ whenever $f, g \in C^\infty(\overline{\Omega})$ are in the domain of $-\Delta_N$ and this motivates the definition of D_N.

Now, let $A = -\sum_{i=1}^n \partial_i^2 : D_N \to L^2(\Omega)$. Our goal is to show that A is essentially self-adjoint and that $\overline{A} = -\Delta_N$. The essential self-adjointness can be seen as follows. Consider the orthonormal sequence $(\psi_k)_{k\in\mathbb{N}_0}$, defined by

$$\psi_0(x) = \frac{1}{\sqrt{2}}, \quad \psi_{2k-1}(x) = \sin\big((k-1/2)\pi x\big), \quad \psi_{2k}(x) = \cos(k\pi x)$$

for $x \in (-1,1)$. Then, a basic fact is that $(\psi_k)_{k\in\mathbb{N}_0}$ lies in $C^\infty([-1;1])$ and forms an orthonormal basis of $L^2((-1,1))$. Morerover, each $\psi_k'(1) = \psi_k'(-1) = 0$ satisfies the Neumann boundary conditions in one dimension. As a consequence, the family

$$\big\{\psi_{j_1,\dots,j_n} = \psi_{j_1}\otimes\psi_{j_2}\otimes\cdots\otimes\psi_{j_n} : j_1,\dots,j_n\in\mathbb{N}_0\big\} \subset D_N \subset L^2(\Omega)$$

is an orthonormal basis of $L^2(\Omega)$ and this set is in fact a subset of D_N (*exercise*). Enumerating the functions by $(\psi_{\mathbf{j}})_{\mathbf{j}\in\mathbb{N}_0^n}$, we obtain an orthonormal eigenbasis of A with

$$A\psi_{\mathbf{j}} = \lambda_{\mathbf{j}}^2\psi_{\mathbf{j}} =: \frac{\pi^2}{4}\sum_{i=1}^n j_i^2\,\psi_{\mathbf{j}}.$$

With this notation, we claim that $\varphi\in D(\overline{A})$ if and only if

$$\sum_{\mathbf{j}\in\mathbb{N}_0^n}\lambda_{\mathbf{j}}^4|\langle\psi_{\mathbf{j}},\varphi\rangle|^2 < \infty. \tag{2.28}$$

Indeed, suppose that (2.28) holds true. Then $\big(\sum_{|\mathbf{j}|\le N}\langle\psi_{\mathbf{j}},\varphi\rangle\psi_{\mathbf{j}}\big)_{N\in\mathbb{N}}$ has the property that $\big(A\sum_{|\mathbf{j}|\le N}\langle\psi_{\mathbf{j}},\varphi\rangle\psi_{\mathbf{j}}\big)_{N\in\mathbb{N}} = \big(\sum_{|\mathbf{j}|\le N}\lambda_{\mathbf{j}}^2\langle\psi_{\mathbf{j}},\varphi\rangle\psi_{\mathbf{j}}\big)_{N\in\mathbb{N}}$ is Cauchy and we have that

$$\lim_{N\to\infty}\Big\|\varphi - \sum_{|\mathbf{j}|\le N}\langle\psi_{\mathbf{j}},\varphi\rangle\psi_{\mathbf{j}}\Big\| = 0,$$

that is, $\varphi\in D(\overline{A})$. On the other hand, if $\varphi\in D(\overline{A})$ and $\zeta\in C_c^\infty(\Omega)\,(\subset D_N)$, we have

$$\langle\zeta,\overline{A}\varphi\rangle = \langle A\zeta,\varphi\rangle = \lim_{N\to\infty}\Big\langle\zeta,\sum_{|\mathbf{j}|\le N}\lambda_{\mathbf{j}}^2\langle\psi_{\mathbf{j}},\varphi\rangle\psi_{\mathbf{j}}\Big\rangle.$$

By density of $C_c^\infty(\Omega)\subset L^2(\Omega)$, this means that $\sum_{|\mathbf{j}|\le N}\lambda_{\mathbf{j}}^2\langle\psi_{\mathbf{j}},\varphi\rangle\varphi_j \rightharpoonup \overline{A}\varphi$ weakly in $L^2(\Omega)$ as $N\to\infty$. Thus, (2.28) holds true and by the previous argument, this implies

$$\overline{A}\varphi = \sum_{\mathbf{j}\in\mathbb{N}_0^n}\lambda_{\mathbf{j}}^2\langle\psi_{\mathbf{j}},\varphi\rangle\psi_{\mathbf{j}}$$

for every $\varphi\in D(\overline{A})$. In other words, $\overline{A}$ is equivalent to a multiplication operator with canonical domain (in the $(\psi_{\mathbf{j}})_{\mathbf{j}\in\mathbb{N}_0^n}$ basis) and hence, $\overline{A}$ is self-adjoint.

In order to show that $\overline{A} = -\Delta_N$, we need to analyze the form q associated to $\overline{A}$. Here, we first recall that for $f,g\in D(A)$, we have by integration by parts that

$$q(f,g) = \int_\Omega dx\,\overline{\nabla f}(x)\cdot\nabla g(x) - \int_{\partial\Omega} d\mathcal{S}\,f\frac{\partial g}{\partial\widehat{n}} = \int_\Omega dx\,\overline{\nabla f}(x)\cdot\nabla g(x).$$

If we denote by q_N the form associated to $-\Delta_N$, this shows that $(q_N)_{|D(A)} = q_{|D(A)}$. Since $D(A)\subset H^1(\Omega)$ is an operator core for $\overline{A}$, it is a form core for q and this implies that $Q(\overline{A})\subset H^1(\Omega)$, recalling that $Q(\overline{A}) = \overline{D(A)}$, the closure being taken with regards to the norm induced by $\langle\cdot,\cdot\rangle_{+1} = q(\cdot,\cdot)+\langle\cdot,\cdot\rangle\big(=\langle\cdot,\cdot\rangle_{H^1(\Omega)}$ on $D(A)\big)$.

What remains to be shown is that $H^1(\Omega) \subset Q(\overline{A})$. So, suppose that $f \in H^1(\Omega)$, then $f \in Q(\overline{A})$ follows if we show that

$$\sum_{\mathbf{j}\in\mathbb{N}_0^n} (1+\lambda_{\mathbf{j}}^2)|\langle \psi_{\mathbf{j}}, f\rangle|^2 \le C\|f\|_{H^1(\Omega)}^2.$$

To prove the latter, suppose that $g \in C^1(\overline{\Omega})$ is such that $g(\pm 1, x_2, \dots, x_n) = 0$. Then

$$\langle \partial_1 f, g\rangle = -\langle f, \partial_1 g\rangle + \int_{\partial\Omega} d\mathcal{S}\, f g\, \widehat{e}_1 \cdot \widehat{n} = -\langle f, \partial_1 g\rangle. \tag{2.29}$$

Here, the integration by parts formula is justified, because $f \in H^1(\Omega)$ admits a trace $f_{|\partial\Omega} \in L^2(\partial\Omega)$, by standard properties of Sobolev functions in the box Ω.

The reason why (2.29) is helpful, is because the functions

$$\big\{\xi_{\mathbf{j}} = \widetilde{\psi}_{j_1} \otimes \psi_{j_2} \otimes \dots \otimes \psi_{j_n} : j_1, \dots, j_n \in \mathbb{N}\big\} \subset C^\infty(\overline{\Omega})$$

for $\widetilde{\psi}_{2k-1}(x) = \cos((k-1/2)\pi x)$, $\widetilde{\psi}_{2k}(x) = \sin(k\pi x)$ are still orthonormal (*exercise*) with

$$\partial_1 \xi_{\mathbf{j}} = \pm\frac{\pi}{2} j_1 \psi_{\mathbf{j}}.$$

Therefore, by Bessel's inequality for orthonormal sequences, we get

$$\sum_{\mathbf{j}\in\mathbb{N}^n} j_1^2 |\langle \psi_{\mathbf{j}}, f\rangle|^2 = \frac{4}{\pi^2}\sum_{\mathbf{j}\in\mathbb{N}^n} |\langle f, \partial_1\xi_{\mathbf{j}}\rangle|^2 = \frac{4}{\pi^2}\sum_{\mathbf{j}\in\mathbb{N}^n} |\langle \partial_1 f, \xi_{\mathbf{j}}\rangle|^2 \le \frac{4}{\pi^2}\|f\|_{H^1(\Omega)}^2$$

and repeating the argument for each coordinate, we conclude that

$$\sum_{\mathbf{j}\in\mathbb{N}_0^n}\Big(1+\frac{\pi^2}{4}\sum_{i=1}^n j_i^2\Big)|\langle \psi_{\mathbf{j}}, f\rangle|^2 = \sum_{\mathbf{j}\in\mathbb{N}_0^n}(1+\lambda_{\mathbf{j}}^2)|\langle \psi_{\mathbf{j}}, f\rangle|^2 \le C\|f\|_{H^1(\Omega)}^2.$$

□

Problem 2.24. *Carry out the proof of part a) of Proposition 2.9.*

Problem 2.25. *For $\Omega = (-1,1)^n$, consider the Laplacian Δ_P with periodic boundary conditions, defined analogously as in Example 2.16. Show that $\Delta_P = \overline{\Delta_{|D_P}}$, where D_P denotes the space of smooth, periodic functions in $\mathbb{R}^n$, that is $D_P = \{f \in C^\infty(\mathbb{R}^n) : f(\cdot) = f(\cdot + p)\,\forall p \in \mathbb{Z}^n\}\big(= C^\infty(\mathbb{T}^n)\big)$.*

2.5.5 Tensor Products of Operators

We finish the chapter about applications of the spectral theorem by collecting some basic properties of tensor products of operators. Throughout this section we assume that A and B are densely defined operators on the Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. Let's denote their domains by $D(A) \subset \mathcal{H}_1$ and $D(B) \subset \mathcal{H}_2$, respectively. We define the space

$$D(A) \otimes D(B) = \operatorname{span}\{\varphi \otimes \psi \in \mathcal{H}_1 \otimes \mathcal{H}_2 : \varphi \in D(A), \psi \in D(B)\}$$

such that $\overline{D(A) \otimes D(B)} = \mathcal{H}_1 \otimes \mathcal{H}_2$. We define $A \otimes B : D(A) \otimes D(B) \to \mathcal{H}_1 \otimes \mathcal{H}_2$ by

$$(A \otimes B)(\varphi \otimes \psi) = A\varphi \otimes B\psi.$$

Lemma 2.11. *$A \otimes B : D(A) \otimes D(B) \to \mathcal{H}_1 \otimes \mathcal{H}_2$ is well-defined, and it is closable whenever $A : D(A) \to \mathcal{H}_1$ and $B : D(B) \to \mathcal{H}_2$ are.*

Proof. Let $f = \sum_{i\in\mathbb{N}} \lambda_i \varphi_i \otimes \psi_i = \sum_{j\in\mathbb{N}} \mu_j \widetilde{\varphi}_j \otimes \widetilde{\psi}_j \in D(A) \otimes D(B)$, with coefficients $\lambda_i, \mu_j \in \mathbb{C}$. By the Gram-Schmidt orthogonalization we can find orthonormal bases of the closures of the spaces $\operatorname{span}\{\varphi_i \in D(A) : i \in \mathbb{N}\} \cup \{\widetilde{\varphi}_i \in D(A) : i \in \mathbb{N}\}$ and $\operatorname{span}\{\psi_j \in D(B) : i \in \mathbb{N}\} \cup \{\widetilde{\psi}_j \in D(B) : i \in \mathbb{N}\}$. Let's denote them by $\{\xi_i \in \mathcal{H}_1 : i \in \mathbb{N}\}$ and $\{\theta_j \in \mathcal{H}_2 : j \in \mathbb{N}\}$, respectively. Then, for all $i, j \in \mathbb{N}$, we have

$$\begin{aligned} \varphi_i \otimes \psi_i &= \sum_{k,l\in\mathbb{N}} \langle \xi_k \otimes \theta_l, \varphi_i \otimes \psi_i \rangle_{\mathcal{H}_1 \otimes \mathcal{H}_2} \xi_k \otimes \theta_l =: \sum_{k,l\in\mathbb{N}} \alpha^i_{kl} \xi_k \otimes \theta_l \\ \widetilde{\varphi}_j \otimes \widetilde{\psi}_j &= \sum_{k,l\in\mathbb{N}} \langle \xi_k \otimes \theta_l, \widetilde{\varphi}_j \otimes \widetilde{\psi}_j \rangle_{\mathcal{H}_1 \otimes \mathcal{H}_2} \xi_k \otimes \theta_l =: \sum_{k,l\in\mathbb{N}} \widetilde{\alpha}^j_{kl} \xi_k \otimes \theta_l \end{aligned}$$

so that, by assumption on f, $\sum_{i\in\mathbb{N}} \lambda_i \alpha^i_{kl} = \sum_{j\in\mathbb{N}} \mu_j \widetilde{\alpha}^j_{kl}$. This shows that

$$\sum_{i\in\mathbb{N}} \lambda_i A\varphi_i \otimes B\psi_i = \sum_{i,k,l\in\mathbb{N}} \lambda_i \alpha^i_{kl} A\xi_k \otimes B\theta_l = \sum_{j,k,l\in\mathbb{N}} \mu_j \widetilde{\alpha}^j_{kl} A\xi_k \otimes B\theta_l = \sum_{j\in\mathbb{N}} \mu_j A\widetilde{\varphi}_i \otimes B\widetilde{\psi}_i$$

so that $A \otimes Bf$ is well-defined. To show that $A \otimes B$ is closable, we only need to show that $D((A \otimes B)^*)$ is dense in $\mathcal{H}_1 \otimes \mathcal{H}_2$, by Theorem 2.2. To this end, we notice that

$$\langle A^* \otimes B^* g, f \rangle_{\mathcal{H}_1 \otimes \mathcal{H}_2} = \langle g, A \otimes Bf \rangle_{\mathcal{H}_1 \otimes \mathcal{H}_2}$$

whenever $g \in D(A^*) \otimes D(B^*)$ and $f \in D(A) \otimes D(B)$. We conclude that $D(A^*) \otimes D(B^*) \subset D((A \otimes B)^*)$ s.t. $D((A \otimes B)^*)$ is dense. □

We define the tensor product of two closable operators $A : D(A) \to \mathcal{H}_1$, $B : D(B) \to \mathcal{H}_2$, as the closure of $A \otimes B : D(A) \otimes D(B) \to \mathcal{H}_1 \otimes \mathcal{H}_2$, and we denote the resulting operator again by $A \otimes B$. Of course, the above generalizes to finitely many tensor products of densely defined operators $A_i : D(A_i) \to \mathcal{H}_i$, $i = 1, \ldots, n \in \mathbb{N}$. The following result characterizes the spectrum of tensor products of operators.

Theorem 2.21. *Let $A_k : D(A_k) \to \mathcal{H}_k$, $k = 1, \ldots, n \in \mathbb{N}$, be self-adjoint operators and let $\mathbb{R}[X_1, \ldots, X_n] \ni P = \sum_{j\in\mathbb{N}_0^n} \lambda_j X_1^{j_1} \ldots X_n^{j_n}$ denote a polynomial in n variables with real coefficients and assume that P has degree l_k in the k-th variable. Suppose that $D_k, k = 1, \ldots, n$, is a domain of essential self-adjointness for $A_k^{l_k}$. Then*

i) $P(A_1, \ldots, A_k) = \sum_{j\in\mathbb{N}_0^n} \lambda_j A_1^{j_1} \otimes A_2^{j_2} \otimes \ldots \otimes A_n^{j_n}$ is essentially self-adjoint on $\bigotimes_{k=1}^n D_k$.

ii) The spectrum of $\overline{P(A_1, \ldots, A_k)}$ is given by

$$\sigma\Big(\overline{P(A_1, \ldots, A_n)}\Big) = \overline{P(\sigma(A_1), \ldots, \sigma(A_n))}$$

Proof. We leave *i*) as an exercise (alternatively, see [55, Sections VII.3 and VIII.10]) and focus on *ii*). By the spectral theorem 2.8, we may assume that each A_k is a multiplication operator that multiplies by a measurable function f_k on an appropriate domain in $L^2(\Omega_k, \mathcal{B}(\Omega_k), \mu_k)$. It is then straightforward - and part of the proof of *i*) - to check (*exercise*) that $\overline{P(A_1, \dots, A_k)}$ is unitarily equivalent to multiplication by

$$\Omega_1 \times \dots \times \Omega_n \ni (x_1, \dots, x_n) \mapsto P(f_1, \dots, f_k)(x_1, \dots, x_n) = \sum_{\mathbf{j} \in \mathbb{N}_0^n} \lambda_{\mathbf{j}} f_1^{j_1}(x_1) \dots f_n^{j_n}(x_n) \in \mathbb{R}$$

on

$$D\Big(\overline{P(A_1, \dots, A_n)}\Big) = \Big\{\varphi \in L^2(\Omega_1 \times \dots \times \Omega_n) : P(f_1, \dots, f_k)\varphi \in L^2(\Omega_1 \times \dots \times \Omega_n)\Big\}$$

where $L^2(\Omega_1 \times \dots \times \Omega_n) = L^2(\Omega_1 \times \dots \times \Omega_n, \otimes_{k=1}^n \mathcal{B}(\Omega_k), \mu = \otimes_{k=1}^n \mu_k)$. The spectrum of $\overline{P(A_1, \dots, A_k)}$ is given by the essential range of $P(f_1, \dots, f_k)$, by Lemma 2.9.

Now, suppose that $\lambda \in P(\sigma(A_1), \dots, \sigma(A_n))$. If $I \subset \mathbb{R}$ is an open interval containing λ, then $P^{-1}(I)$ contains a product $I_1 \times \dots \times I_n \subset \mathbb{R}^n$ of open intervals $I_k \subset \mathbb{R}$ with $I_k \cap \sigma(A_k) \neq \emptyset$. Since $\sigma(A_k) = \text{ess-ran}(f_k)$, we have $\mu_k(f_k^{-1}(I_k)) > 0$ such that

$$\mu\big(P(f_1, \dots, f_n)^{-1}(I)\big) \geq \mu\Big(f_1^{-1}(I_1) \times \dots \times f_n^{-1}(I_n)\Big) \geq \prod_{k=1}^n \mu_k(f_k^{-1}(I_k)) > 0.$$

Since I was arbitrary, this implies that $P(\sigma(A_1), \dots, \sigma(A_n)) \subset \sigma\big(\overline{P(A_1, \dots, A_n)}\big)$ and thus, by closedness of the spectrum, that $\overline{P(\sigma(A_1), \dots, \sigma(A_n))} \subset \sigma\big(\overline{P(A_1, \dots, A_n)}\big)$. On the other hand, if $\lambda \notin \overline{P(\sigma(A_1), \dots, \sigma(A_n))}$, then $(P(f_1, \dots, f_n) - \lambda)^{-1}$ is a bounded, measurable function so that $\lambda \in \rho\big(\overline{P(A_1, \dots, A_n)}\big)$. □

Problem 2.26. *Let $A : D(A) \to \mathcal{H}$ be self-adjoint and let $P(A)$, for some real polynomial $P[X]$ of degree $d \in \mathbb{N}$, as a self-adjoint operator on its canonical domain. Show that every core D of A^d is a core for $P(A)$. Generalize the proof to conclude Theorem 2.21 i).*

Problem 2.27. *Consider $\Omega = (-\frac{1}{2}, \frac{1}{2})^n$ and let Δ_D, Δ_N and Δ_P denote the Dirichlet-, Neumann- and, respectively, periodic Laplacian, defined on suitable domains in $L^2(\Omega)$. For each case, determine the spectrum of the many-body kinetic energy operator*

$$\sum_{i=1}^N (-\Delta_{x_i}).$$

Here, $\Delta_{x_i} = \mathbf{1} \otimes \dots \otimes \Delta \otimes \dots \mathbf{1}$ and Δ acts on the i-th factor in $L^2(\Omega^N) = \bigotimes_{i=1}^N L^2(\Omega)$.

2.6 Selected Tools for Complete BEC

In this section we introduce some additional tools that are directly related to the concept of Bose-Einstein condensation. We introduce the trace and the Hilbert Schmidt classes and summarize some of their basic properties. Equipped with these basics on trace class operators, we introduce the notion of complete Bose-Einstein condensation.

2.6.1 Trace Class and Hilbert-Schmidt Operators

The trace class and Hilbert-Schmidt are subspaces of the (Banach) space of compact operators on a Hilbert space $\mathcal{H}$. Recall that every compact operator admits a representation in terms of its singular values: defining the absolute value of A by

$$|A| = \sqrt{A^*A} \in \mathcal{L}(\mathcal{H}),$$

and denoting by $(\lambda_n)_{n\in\mathbb{N}}$ its eigenvalues, one finds orthonormal sequences $(\varphi_n)_{n\in\mathbb{N}}$, $(\psi_n)_{n\in\mathbb{N}}$ such that

$$A = \sum_{n\in\mathbb{N}} \lambda_n |\varphi_n\rangle\langle\psi_n|,$$

where we recall that $|\varphi\rangle\langle\psi|$ denotes the rank-one operator defined by $|\varphi\rangle\langle\psi|\zeta = \langle\psi,\zeta\rangle\varphi$.

Problem 2.28. *Let $A \in \mathcal{L}(\mathcal{H})$ and suppose $A \geq 0$. Prove that its square-root $\sqrt{A}$ is unique, that is, there exists a unique $B \in \mathcal{L}(\mathcal{H})$, $B \geq 0$, such that $B^2 = A$.*

Problem 2.29. *Let $A \in \mathcal{L}(\mathcal{H})$ be compact. Show that $|A|$ is compact as well.*

The trace class and Hilbert-Schmidt operators are those compact operators whose sequence of singular values lies in ℓ^1 and ℓ^2, respectively. To study some of the basic properties of these classes, we start with a useful lemma: similar to the decomposition $z = |z|e^{i\arg(z)}$ for any complex number $z \in \mathbb{C}$, we can decompose bounded operators.

Lemma 2.12 (Polar Decomposition)**.** *Let $A \in \mathcal{L}(\mathcal{H})$. Then, there exists a partial isometry $U \in \mathcal{L}(\mathcal{H})$ s.t. $A = U|A|$ and U is uniquely determined by $\ker(U) = \ker(A)$.*

Proof. Define the map $U : \operatorname{ran}(|A|) \to \operatorname{ran}(A)$ by setting $U(|A|\psi) = A\psi$. We have

$$\||A|\psi\|_{\mathcal{H}}^2 = \langle\psi, A^*A\psi\rangle_{\mathcal{H}} = \|A\psi\|_{\mathcal{H}}^2 = \|U|A|\psi\|_{\mathcal{H}}^2$$

so that $U : \operatorname{ran}(|A|) \to \operatorname{ran}(A)$ is well-defined and an isometry. Due to the last fact, we can extend it to $U : \overline{\operatorname{ran}(|A|)} \to \overline{\operatorname{ran}(A)}$. We then set U equal to zero in $\overline{\operatorname{ran}(|A|)}^{\perp}$. Notice that $\overline{\operatorname{ran}(|A|)}^{\perp} = \ker(|A|) = \ker(A)$, since $|A|$ is self-adjoint. Thus, $\ker(U) = \ker(A)$. Finally, given another partial isometry $\widetilde{U}$ s.t. $A = \widetilde{U}|A|$ and $\ker(\widetilde{U}) = \ker(A)$, we have $\widetilde{U} - U = 0$ on $\overline{\operatorname{ran}(|A|)}$ and on $\ker(A) = \overline{\operatorname{ran}(|A|)}^{\perp}$, i.e. $\widetilde{U} = U$. □

Problem 2.30. *Generalize Lemma 2.12 to the case where $A : D(A) \to \mathcal{H}$ is a densely defined, closed operator. In this case, the difficulty is to construct $|A| = \sqrt{A^*A}$, because a priori it is not even clear that A^*A is densely defined. Use a quadratic form argument to show that A^*A is indeed densely defined and self-adjoint (it suffices to show that A^*A is a symmetric extension of a suitable self-adjoint operator).*

The polar decomposition turns out to be useful when studying some properties of the trace class and Hilbert-Schmidt operators with which we start now. As mentioned earlier, the trace class is a subclass of the compact operators s.t. their sequence of singular values lies in ℓ^1. To make this more precise, we introduce first the trace of a positive operator. Given any $A \in \mathcal{L}(\mathcal{H})$ s.t. $A \geq 0$ and an orthonormal basis $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$ of the Hilbert space $\mathcal{H}$, we define the trace of A by

$$\operatorname{tr} A = \sum_{n \in \mathbb{N}} \langle \varphi_n, A\varphi_n \rangle_{\mathcal{H}} \in [0, \infty].$$

The following proposition shows in particular that the trace is well-defined.

Lemma 2.13. *Let $A, B \in \mathcal{L}(H)$ be non-negative, let $\lambda, \mu \in \mathbb{C}$ and suppose that $U \in \mathcal{L}(\mathcal{H})$ is unitary. Then the following holds true.*

i) $\operatorname{tr} A$ *is independent of the chosen basis* $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$.

ii) $\operatorname{tr}(\lambda A + \mu B) = \lambda \operatorname{tr} A + \mu \operatorname{tr} B$.

iii) $\operatorname{tr} UAU^{-1} = \operatorname{tr} A$.

Proof. Denote by $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$, $\{\psi_n \in \mathcal{H} : n \in \mathbb{N}\}$ any two bases of $\mathcal{H}$. Then

$$\begin{aligned}\sum_{k \in \mathbb{N}} \langle \varphi_k, A\varphi_k \rangle_{\mathcal{H}} = \sum_{k \in \mathbb{N}} \Big(\sum_{l \in \mathbb{N}} |\langle \psi_l, A^{1/2}\varphi_k \rangle_{\mathcal{H}}|^2 \Big) &= \sum_{k \in \mathbb{N}} \Big(\sum_{l \in \mathbb{N}} |\langle A^{1/2}\psi_l, \varphi_k \rangle_{\mathcal{H}}|^2 \Big) \\ &= \sum_{l \in \mathbb{N}} \langle \psi_l, A\psi_l \rangle_{\mathcal{H}}\end{aligned}$$

This proves that $\operatorname{tr} A$ is independent of the basis. Linearity of the trace is a simple exercise and part *iii*) follows due to the fact that $\{U^{-1}\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$ is a basis of $\mathcal{H}$ whenever $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$ is if $U \in \mathcal{L}(\mathcal{H})$ is unitary. □

We define the trace class $\mathcal{J}_1$ as the set

$$\mathcal{J}_1 = \{A \in \mathcal{L}(\mathcal{H}) : \operatorname{tr} |A| < \infty\}.$$

Below $\mathcal{J}_1$ turns out to be a Banach space when equipped with a suitable norm.

Proposition 2.10. *$\mathcal{J}_1$ is a *-ideal in $\mathcal{L}(\mathcal{H})$, meaning that*

i) $\mathcal{J}_1$ is a vector space.

ii) If $A \in \mathcal{J}_1$ and $B \in \mathcal{L}(\mathcal{H})$, then $AB \in \mathcal{J}_1$ and $BA \in \mathcal{J}_1$.

iii) If $A \in \mathcal{J}_1$, then $A^* \in \mathcal{J}_1$.

Proof. i) It is clear that $\mathcal{J}_1$ is closed under scalar multiplication, since $|\lambda A| = |\lambda||A|$ for any $\lambda \in \mathbb{C}$, $A \in \mathcal{L}(\mathcal{H})$. To prove that $A + B \in \mathcal{J}_1$ whenever $A, B \in \mathcal{J}_1$, we make use of Lemma 2.12. Suppose that $A + B = U|A + B|$, $A = V|A|$ and $B = W|B|$ for partial isometries $U, V, W \in \mathcal{L}(\mathcal{H})$ and let $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$ be an orthonormal basis of $\mathcal{H}$. Then, by Cauchy-Schwarz,

$$\begin{aligned}\operatorname{tr}|A+B| =& \sum_{n=1}^{\infty}\langle\varphi_n, U^*V|A|\varphi_n\rangle_{\mathcal{H}} + \sum_{n=1}^{\infty}\langle\varphi_n, U^*W|B|\varphi_n\rangle_{\mathcal{H}} \\ \leq& (\operatorname{tr}|A|)^{1/2}\Big(\sum_{n=1}^{\infty}\langle\varphi_n, U^*V|A|V^*U\varphi_n\rangle_{\mathcal{H}}\Big)^{1/2} \\ &+ (\operatorname{tr}|B|)^{1/2}\Big(\sum_{n=1}^{\infty}\langle\varphi_n, U^*W|B|W^*U\varphi_n\rangle_{\mathcal{H}}\Big)^{1/2}\end{aligned}$$

Now, U, V, W are partial isometries and, by Lemma 2.13, taking traces is independent of the chosen basis. Therefore, we deduce

$$\operatorname{tr}|A+B| \leq \operatorname{tr}|A| + \operatorname{tr}|B|$$

which concludes the proof that $\mathcal{J}_1$ is a vector space.

ii) Suppose first that $U \in \mathcal{L}(\mathcal{H})$ is a unitary operator. Then $|UA| = \sqrt{A^*U^*UA} = |A|$ and $|AU| = U^*|A|U$ (recall here that the square root is unique by Problem 2.28). Therefore, $UA \in \mathcal{J}_1$ and $AU \in \mathcal{J}_1$, whenever $A \in \mathcal{J}_1$.

Now, let $B \in \mathcal{L}(\mathcal{H})$. Such operators can be written as a linear combination of four unitary operators, which proves *ii)* by applying *i)*. To prove that B can be written as such a linear combination, we note first that B can be written as a linear combination of two self-adjoint operators. More precisely, we have

$$B = \frac{1}{2}(B + B^*) + \frac{i}{2}(iB^* - iB)$$

If $0 \neq C \in \mathcal{L}(\mathcal{H})$ is self-adjoint, on the other hand, it is equal to $C = \widetilde{C}\|C\|_{\mathcal{L}(\mathcal{H})}$ where

$$\widetilde{C} = \frac{1}{2}\Big[\widetilde{C} + i(1-\widetilde{C}^2)^{1/2}\Big] + \frac{1}{2}\Big[\widetilde{C} - i(1-\widetilde{C}^2)^{1/2}\Big]$$

is the linear combination of two unitary operators.

iii) We write $A = U|A|$ for a partial isometry $U \in \mathcal{L}(\mathcal{H})$, by Lemma 2.12. If $A \in \mathcal{J}_1$, then clearly $|A| \in \mathcal{J}_1$. But then also $A^* = |A|U^* \in \mathcal{J}_1$, by *ii)*. □

Remark 2.3. *One might be tempted to use $|A+B| \leq |A| + |B|$ in order to show that $\operatorname{tr}|A+B| \leq \operatorname{tr}|A| + \operatorname{tr}|B|$. However, the first inquality is in general not true. Consider the following example due to E. Nelson (see Problem 16 in [55, Chapter VI]). Define*

$$A = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$$

Then

$$|A| + |B| = \begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix}, \qquad |A+B| = \begin{pmatrix} \sqrt{2} & 0 \\ 0 & \sqrt{2} \end{pmatrix}$$

so that $\langle\varphi, |A+B|\varphi\rangle_{\mathbb{C}^2} > \langle\varphi, (|A|+|B|)\varphi\rangle_{\mathbb{C}^2}$ for $\varphi = (0\ \ 1) \in \mathbb{C}^2$.

Theorem 2.22. *Define* $\|A\|_{\mathcal{J}_1} = \operatorname{tr}|A|$ *for* $A \in \mathcal{J}_1$. *Then* $(\mathcal{J}_1, \|\cdot\|_{\mathcal{J}_1})$ *is a Banach space and* $\|A\|_{\mathcal{L}(\mathcal{H})} \leq \|A\|_{\mathcal{J}_1}$ *for all* $A \in \mathcal{J}_1$. *Moreover, any* $A \in \mathcal{J}_1$ *is compact and a compact operator lies in* $\mathcal{J}_1$ *if and only if the sequence of its singular values lies in* ℓ^1.

Proof. The proof of Proposition 2.10 has shown that $\|\cdot\|_{\mathcal{J}_1}$ defines a norm on $\mathcal{J}_1$. That $\|A\|_{\mathcal{L}(\mathcal{H})} \leq \|A\|_{\mathcal{J}_1}$ for all $A \in \mathcal{J}_1$ follows from the fact that $\|A\|_{\mathcal{L}(\mathcal{H})} = \||A|\|_{\mathcal{L}(\mathcal{H})}$ and

$$\||A|\|_{\mathcal{L}(\mathcal{H})} = \sup_{\varphi \in \mathcal{H}, \|\varphi\|_{\mathcal{H}}=1} \langle \varphi, |A|\varphi\rangle \leq \operatorname{tr}|A|$$

where we used that $|A| \in \mathcal{L}(\mathcal{H})$ is self-adjoint. Now, assume that $(A_n)_{n\in\mathbb{N}}$ is Cauchy in $\mathcal{J}_1$. Since the $\mathcal{J}_1$-norm dominates the $\mathcal{L}(\mathcal{H})$-norm, $(A_n)_{n\in\mathbb{N}}$ converges in particular to some $A \in \mathcal{L}(\mathcal{H})$. Writing $A = U|A|$ and $A_n = U_n|A_n|$ for partial isometries $U, U_n, n \in \mathbb{N}$, by Lemma 2.12, we have for any orthonormal basis $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$ and $N \in \mathbb{N}$ that

$$\sum_{n=1}^{N} \langle \varphi_n, |A|\varphi_n\rangle_{\mathcal{H}} = \lim_{k\to\infty} \sum_{n=1}^{N} \langle \varphi_n, U^* U_k |A_k|\varphi_n\rangle_{\mathcal{H}} \leq \sup_{k\in\mathbb{N}} \operatorname{tr}|A_k| = \sup_{k\in\mathbb{N}} \|A_k\|_{\mathcal{J}_1} < \infty$$

Letting $N \to \infty$, this proves that $A \in \mathcal{J}_1$. Arguing similarly for $\sum_{n=1}^{N} \langle \varphi_n, |A - A_k|\varphi_n\rangle_{\mathcal{H}}$ shows that $\lim_{k\to\infty} \|A - A_k\|_{\mathcal{J}_1} = 0$. Hence, $(\mathcal{J}_1, \|\cdot\|_{\mathcal{J}_1})$ is a Banach space.

To show that $\mathcal{J}_1$ is a subset of the set of compact operators, we show that any $A \in \mathcal{J}_1$ is the norm limit of a finite rank operator. To this end, let $A \in \mathcal{J}_1$. By Proposition 2.10 *ii*), also $|A|^2 \in \mathcal{J}_1$ so that $\operatorname{tr}|A|^2 < \infty$. Now, given an orthonormal basis $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$ and a state $\psi \in \{\varphi_1, \ldots, \varphi_N\}^\perp$ with $\|\psi\| \leq 1$, we conclude that

$$\begin{aligned}\|A\psi\|_{\mathcal{H}}^2 &= \sum_{k,l>N} \langle \psi, \varphi_k\rangle_{\mathcal{H}} \langle \varphi_k, |A|^2\varphi_l\rangle_{\mathcal{H}} \langle \varphi_l, \psi\rangle_{\mathcal{H}} \\ &\leq \operatorname{tr}|A|^2 - \sum_{n=1}^{N} \langle \varphi_n, |A|^2\varphi_n\rangle_{\mathcal{H}} \to 0\end{aligned}$$

as $N \to \infty$, uniformly over $\|\psi\| \leq 1$. This implies that

$$\begin{aligned}0 = \lim_{N\to\infty} \sup_{\substack{\psi\in\{\varphi_1,\ldots,\varphi_N\}^\perp,\\ \|\psi\|_{\mathcal{H}}\leq 1}} \|A\psi\|_{\mathcal{H}} &= \lim_{N\to\infty} \sup_{\substack{\xi\in\mathcal{H},\\ \|\xi\|_{\mathcal{H}}\leq 1}} \Big\|A\big(\xi - \sum_{n=1}^{N} |\varphi_n\rangle\langle\varphi_n|\big)\xi\Big\|_{\mathcal{H}} \\ &= \lim_{N\to\infty} \sup_{\substack{\xi\in\mathcal{H},\\ \|\xi\|_{\mathcal{H}}\leq 1}} \Big\|\big(A - \sum_{n=1}^{N} |A\varphi_n\rangle\langle\varphi_n|\big)\xi\Big\|_{\mathcal{H}},\end{aligned}$$

from which we conclude that $A \in \mathcal{J}_1$ is compact.

Finally, notice that $A \in \mathcal{J}_1$ if and only if $|A| \in \mathcal{J}_1$ and that the singular values of A are the eigenvalues of $|A|$, which is self-adjoint. Since compact, self-adjoint operators admit an eigenbasis which is a complete orthonormal basis of $\mathcal{H}$, it follows that a compact operator $A \in \mathcal{L}(\mathcal{H})$ lies in $\mathcal{J}_1$ if and only if its sequence of singular values lies in ℓ^1. $\square$

In analogy to the properties of the Lebesgue-integrable functions, we can now define the trace of a trace class operator (so far, it was only defined for positive operators).

Proposition 2.11. *Let $A \in \mathcal{J}_1$ and assume that $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$ is an orthonormal basis of $\mathcal{H}$. Then, the sum $\sum_{n=1}^{\infty} \langle \varphi_n, A\varphi_n \rangle_{\mathcal{H}}$ converges absolutely and is independent of the chosen basis $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$.*

Remark 2.4. *We call* $\mathrm{tr} : \mathcal{J}_1 \to \mathbb{C}$ *where* $\mathrm{tr}\, A = \sum_{n=1}^{\infty} \langle \varphi_n, A\varphi_n \rangle_{\mathcal{H}}$*, the trace.*

Proof. We write $A = U|A| = U|A|^{1/2}|A|^{1/2}$. The absolute convergence follows from

$$\sum_{n=1}^{\infty} |\langle \varphi_n, A\varphi_n \rangle_{\mathcal{H}}| \leq \left(\sum_{n=1}^{\infty} \| |A|^{1/2} U^* \varphi_n \|_{\mathcal{H}}^2 \right)^{1/2} \left(\sum_{n=1}^{\infty} \| |A|^{1/2} \varphi_n \|_{\mathcal{H}}^2 \right)^{1/2} \leq \mathrm{tr}\, |A|.$$

The independence of the basis follows similarly as in the proof of Lemma 2.13. □

Problem 2.31. *In Proposition 2.10, we have seen that $\mathcal{J}_1$ is an ideal, meaning that $AB \in \mathcal{J}_1$ and $BA \in \mathcal{J}_1$ if $A \in \mathcal{J}_1$ and $B \in \mathcal{L}(\mathcal{H})$. Prove that*

$$\mathrm{tr}\, |BA| = \mathrm{tr}\, |AB| \leq \|B\|_{\mathcal{L}(\mathcal{H})} \mathrm{tr}\, |A|.$$

Hint: Prove first that $A \geq B$ implies $\sqrt{A} \geq \sqrt{B}$ using the functional calculus.

Problem 2.32. *Suppose that $\varphi \in L^2(\mathbb{R}^d)$, $\|\varphi\| = 1$, and $v \in L^\infty(\mathbb{R}^d)$ such that $0 \leq \widehat{v} \in L^1(\mathbb{R}^d)$ (here, $\widehat{v}$ denotes the distributional Fourier transform of v, viewed as a tempered distribution). Show that the operator K, defined by its integral kernel*

$$K(x, y) = \overline{\varphi}(x) v(x - y) \varphi(y),$$

is a non-negative trace class operator $K \in \mathcal{J}_1$ and find its trace.

Problem 2.33. *Show that $A \in \mathcal{J}_1$ if and only if $\sum_{n=1}^{\infty} |\langle \varphi_n, A\varphi_n \rangle| < \infty$ for every orthonormal basis $(\varphi_n)_{n \in \mathbb{N}}$. Find an example of an operator $B \notin \mathcal{J}_1$ and an ONB $(\psi_n)_{n \in \mathbb{N}}$ such that $\sum_{n=1}^{\infty} |\langle \psi_n, B\psi_n \rangle| < \infty$.*

Proposition 2.12. *Denote by $\mathcal{C}(\mathcal{H})$ the set of compact operators on $\mathcal{H}$, which is a closed subset of $\mathcal{L}(\mathcal{H})$. Then the following holds true.*

i) The map $\mathcal{J}_1 \ni A \mapsto \mathrm{tr}(A\,\cdot) \in \mathcal{C}(\mathcal{H})^*$ is an isometric isomorphism s.t. $\mathcal{C}(\mathcal{H})^* \simeq \mathcal{J}_1$.

ii) The map $\mathcal{L}(\mathcal{H}) \ni B \mapsto \mathrm{tr}(B\,\cdot) \in \mathcal{J}_1^*$ is an isometric isomorphism s.t. $\mathcal{J}_1^* \simeq \mathcal{L}(\mathcal{H})$.

Proof. We focus *i)* and leave *ii)* as an *exercise*. Let $f \in \mathcal{C}(\mathcal{H})^*$, $\varphi, \psi \in \mathcal{H}$ and define the compact rank-one operator $l_{\psi,\varphi} \in \mathcal{C}(\mathcal{H})$ by

$$l_{\psi,\varphi} = |\varphi\rangle\langle\psi|.$$

The key step is to express $f(|\varphi\rangle\langle\psi|)$ as a trace of $|\varphi\rangle\langle\psi|$ against some trace class operator. Here, we use Riesz' lemma: the map $\psi \mapsto l_{\psi,\varphi} \in C(\mathcal{H})$ is conjugate linear so that the map $j_\varphi : \mathcal{H} \to \mathbb{C}$, defined by

$$\psi \mapsto j_\varphi(\psi) = \overline{f(l_{\psi,\varphi})}$$

is a bounded, linear map $j_\varphi \in \mathcal{H}^*$. Indeed, we have that $\|j_\varphi\|_{\mathcal{H}^*} \leq \|f\|_{\mathcal{C}(\mathcal{H})^*}\|\varphi\|_{\mathcal{H}}$. By Riesz' lemma, there exists a unique $\zeta_\varphi \in \mathcal{H}$ such that

$$j_\varphi = \langle \zeta_\varphi, \cdot \rangle_{\mathcal{H}}$$

with $\|\zeta_\varphi\|_{\mathcal{H}} = \|j_\varphi\|_{\mathcal{H}^*}$. Using ζ_φ, we define a linear operator $B : \mathcal{H} \to \mathcal{H}$ by

$$B\varphi = \zeta_\varphi$$

such that we have for all $\psi, \varphi \in \mathcal{H}$

$$\operatorname{tr}\big(|\varphi\rangle\langle\psi|B\big) = \langle \psi, B\varphi\rangle_{\mathcal{H}} = \langle \psi, \zeta_\varphi\rangle_{\mathcal{H}} = f(l_{\psi,\varphi}) = f\big(|\varphi\rangle\langle\psi|\big).$$

It is simple to check that B is indeed linear and from $\|\zeta_\varphi\|_{\mathcal{H}} = \|j_\varphi\|_{\mathcal{H}^*} \leq \|f\|_{\mathcal{C}(\mathcal{H})^*}\|\varphi\|_{\mathcal{H}}$, we get $\|B\|_{\mathcal{L}(\mathcal{H})} \leq \|f\|_{\mathcal{C}(\mathcal{H})^*}$. Writing $B = U|B|$, by Lemma 2.12, we observe that

$$\sum_{n=1}^{N} \langle \varphi_n, |B|\varphi_n\rangle_{\mathcal{H}} = \sum_{n=1}^{N} \langle U\varphi_n, B\varphi_n\rangle_{\mathcal{H}} = f\bigg(\sum_{n=1}^{N} |\varphi_n\rangle\langle U\varphi_n|\bigg)$$

for every ONB $\{\varphi_k : k \in \mathbb{N}\}$ of $\mathcal{H}$. Using that U is a partial isometry, we get

$$\Big\| \sum_{n=1}^{N} \langle U\varphi_n, \cdot\rangle_{\mathcal{H}}\, \varphi_n \Big\|_{\mathcal{L}(\mathcal{H})}^2 = \sup_{\xi\in\mathcal{H}, \|\xi\|_{\mathcal{H}}=1} \Big\langle \sum_{n=1}^{N} \langle U\varphi_n, \xi\rangle_{\mathcal{H}}\, \varphi_n, \sum_{m=1}^{N} \langle U\varphi_m, \xi\rangle_{\mathcal{H}}\, \varphi_m \Big\rangle_{\mathcal{H}} \leq 1$$

and hence $B \in \mathcal{J}_1$ with $\|B\|_{\mathcal{J}_1} \leq \|f\|_{\mathcal{C}(\mathcal{H})^*}$. Moreover, we find that

$$f(T) = \operatorname{tr}(BT)$$

for all $T \in \mathcal{C}(\mathcal{H})$ using that $f(|\varphi\rangle\langle\psi|) = \langle\psi, B\varphi\rangle_{\mathcal{H}} = \operatorname{tr}(B|\varphi\rangle\langle\psi|)$ and density of the finite rank operators in the space of compact operators. This shows that

$$\|B\|_{\mathcal{J}_1} \leq \|f\|_{\mathcal{C}(\mathcal{H})^*} = \sup_{T\in\mathcal{C}(\mathcal{H}), \|T\|_{\mathcal{L}(\mathcal{H})}=1} |\operatorname{tr}(BT)| \leq \|B\|_{\mathcal{J}_1}$$

and it implies that $\mathcal{J}_1 \ni A \mapsto \operatorname{tr}(A\,\cdot) \in \mathcal{C}(\mathcal{H})^*$ is an isometric isomorphism. □

Before closing this section, we briefly introduce another important operator class, the Hilbert-Schmidt class. While $\mathcal{J}_1$ is the operator class analogue of ℓ^1, the Hilbert-Schmidt class is the analogue of ℓ^2: we call $A \in \mathcal{L}(\mathcal{H})$ a Hilbert-Schmidt operator if

$$\operatorname{tr} A^*A < \infty \quad \Longleftrightarrow \quad |A|^2 \in \mathcal{J}_1.$$

Theorem 2.23. *Let $\mathcal{J}_2 = \{A \in \mathcal{L}(\mathcal{H}) : \operatorname{tr} A^*A < \infty\}$ denote the set of Hilbert-Schmidt operators. Then the following holds true.*

i) $\mathcal{J}_2$ is a *-ideal.

ii) Defining $\langle A, B\rangle_{\mathcal{J}_2} = \sum_{n=1}^{\infty} \langle \varphi_n, A^*B, \varphi_n\rangle_{\mathcal{H}}$ for every $A, B \in \mathcal{J}_2$, then $\langle A, B\rangle_{\mathcal{J}_2}$ is absolutely summable and independent of the chosen basis.

iii) $(\mathcal{J}_2, \langle\cdot,\cdot\rangle_{\mathcal{J}_2})$ is a Hilbert space and $\|A\|_{\mathcal{L}(\mathcal{H})} \le \|A\|_{\mathcal{J}_2} \le \|A\|_{\mathcal{J}_1}$ for every $A \in \mathcal{L}(\mathcal{H})$.

iv) Every $A \in \mathcal{J}_2$ is compact and a compact operator lies in $\mathcal{J}_2$ if and only if its sequence of singular values lies in ℓ^2.

Proof. The proof uses very similar arguments as in the proofs of Proposition 2.10 and Theorem 2.22. We leave it as an *exercise.* □

Since we typically work in the L^2 setting, it is useful to observe that Hilbert-Schmidt operators have a concrete realization in this case.

Proposition 2.13. *Consider the Hilbert space $\mathcal{H} = L^2(\Omega, \mathcal{A}, \mu)$. Then $A \in \mathcal{J}_2$ if and only if there exists an element $K \in L^2(\Omega \times \Omega, \mathcal{A} \otimes \mathcal{A}, \mu \otimes \mu)$ such that A is equal to the integral operator acting on $f \in L^2(\Omega, \mathcal{A}, \mu)$ by*

$$(Af)(x) = \int_\Omega K(x; y) f(y)\, d\mu(y) \quad \text{for } \mu \text{ a.e. } x \in \Omega.$$

Moreover, in this case we have $\|A\|^2_{\mathcal{J}_2} = \int_{\Omega\times\Omega} |K(x; y)|^2\, d\mu(x)d\mu(y)$.

Proof. Denote by A_K the integral operator associated with $K \in L^2(\Omega\times\Omega, \mathcal{A}\otimes\mathcal{A}, \mu\otimes\mu)$. For any $f \in L^2(\Omega, \mathcal{A}, \mu)$, a simple application of Cauchy-Schwarz and Fubini implies

$$\begin{aligned}&\int_\Omega \Big(\int_\Omega \overline{K(x;y)f(y)}\, d\mu(y)\Big)\Big(\int_\Omega K(x;z)f(z)\, d\mu(z)\Big) d\mu(x)\\ &\quad\le \int_{\Omega\times\Omega\times\Omega} |K(x;y)||f(z)||K(x;z)||f(y)|\, d\mu(x)d\mu(y)d\mu(z) \le \|K\|^2_{L^2(\Omega\times\Omega)}\|f\|^2_{L^2(\Omega)}\end{aligned}$$

Hence, A_K is a bounded operator in $L^2(\Omega, \mathcal{A}, \mu)$ with $\|A_K\|_{\mathcal{L}(\mathcal{H})} \le \|K\|_{L^2(\Omega\times\Omega)}$. Now let $\{\varphi_n \in \mathcal{H} : n \in \mathbb{N}\}$ be an orthonormal basis of $L^2(\Omega, \mathcal{A}, \mu)$. Then $\{\varphi_m \otimes \overline{\varphi}_n \in \mathcal{H}\otimes\mathcal{H} : m, n \in \mathbb{N}\}$ is a basis of $L^2(\Omega \times \Omega, \mathcal{A} \otimes \mathcal{A}, \mu \otimes \mu)$ so that

$$K = \sum_{n,m=1}^{\infty} K_{mn}\, \varphi_m \otimes \overline{\varphi}_n, \qquad K_{mn} = \langle \varphi_m \otimes \overline{\varphi}_n, K\rangle_{L^2(\Omega\times\Omega} \ \ (\forall\, m, n \in \mathbb{N})$$

Define $K_N \in L^2(\Omega \times \Omega, \mathcal{A} \otimes \mathcal{A}, \mu \otimes \mu)$ by $K_N = \sum_{m,n=1}^{N} K_{mn}\varphi_m \otimes \overline{\varphi}_n$. Then K_N is the operator kernel of $A_{K_N} \in \mathcal{L}(\mathcal{H})$, defined by $A_{K_N} = \sum_{m,n=1}^{N} K_{mn}|\varphi_m\rangle\langle\varphi_n|$. Since

$\lim_{N\to\infty} \|K - K_N\|_{L^2(\Omega\times\Omega)} = 0$, the first step implies that $\lim_{N\to\infty} \|A_K - A_{K_N}\|_{\mathcal{L}(\mathcal{H})} = 0$. This implies that A_K is compact and we find furthermore that

$$\operatorname{tr} A_K^* A_K = \sum_{n=1}^{\infty} \|A_K\varphi_n\|_2^2 = \sum_{m,n=1}^{\infty} |\langle \varphi_m, A_K\varphi_n\rangle_2|^2 = \sum_{m,n=1}^{\infty} |\langle \varphi_m \otimes \overline{\varphi}_n, K\rangle_{L^2(\Omega\times\Omega)}|^2$$
$$= \|K\|_{L^2(\Omega\times\Omega)}^2 < \infty$$

This implies that the map $\Phi : L^2(\Omega \times \Omega, \mathcal{A}\otimes\mathcal{A}, \mu\otimes\mu) \to \mathcal{J}_2$, given by $K \mapsto A_K$, is an isometry. In particular, it has a closed range. Moreover, any finite rank operator can be represented as an integral operator with kernel in $L^2(\Omega \times \Omega, \mathcal{A}\otimes\mathcal{A}, \mu\otimes\mu)$, so that the range of Φ contains the finite rank operators. These operators are dense in $\mathcal{J}_2$, which follows for instance by approximating $A \in \mathcal{J}_2$ by the sequence $(A_N)_{N\in\mathbb{N}}$

$$A_N = \sum_{n,m=1}^{N} \langle \varphi_m, A\varphi_n\rangle |\varphi_n\rangle\langle\varphi_m|.$$

□

2.6.2 Complete Bose-Einstein Condensation

In this section, we define the notion of (asymptotically) complete Bose-Einstein condensation. There are different notions of Bose-Einstein condensation in the literature, but the one introduced here is the one with which we work in the following sections.

As motivated in Section 1, we consider N bosons moving in some region $\Omega \subset \mathbb{R}^3$. The system is described by a wave function $\psi_N \in L_s^2(\Omega^N, \mathcal{B}(\Omega^N), \otimes_{j=1}^N \mu) = L_s^2(\Omega^N) = \mathcal{H}^{\otimes_s N}$, where $\mathcal{H} = L_s^2(\Omega)$. We saw in Section 1 that Bose-Einstein condensation can be understood as the property that, in the limit of large N, a macroscopic fraction of particles occupies the same one particle wave function. However, typical wave functions of interest, like the ground state wave function of a many body Schrödinger operator with non-vanishing interaction potential, are not equal to pure tensor products. So, we need to specify what we actually mean if we say that a macroscopic fraction of the particles of the many body wave function occupies the same one-particle wave function. The appropriate object that gives precise meaning to the latter idea, is the so called one-particle reduced density matrix. Given a normalized wave function $\psi_N \in L_s^2(\Omega^N)$, the associated one-particle reduced density matrix $\gamma_N^{(1)} \in \mathcal{J}_1$ is the positive trace class operator with integral kernel

$$\gamma_N^{(1)}(x,y) = \int_{\Omega^{N-1}} \psi_N(x, x_2, \dots, x_N)\overline{\psi}_N(y, x_2, \dots, x_N)\, dx_2 \dots dx_N$$

It is clear that $\langle \varphi, \gamma_N^{(1)}\varphi\rangle_2 \geq 0$ and, applying Plancherel and Fubini, we also see that

$$\operatorname{tr} \gamma_N^{(1)} = \sum_{n=1}^{\infty} \int_{\Omega^{N-1}} |\langle \varphi_n, \psi_N(\cdot\,, X)\rangle_2|^2\, dX = \int_{\Omega^{N-1}} \|\psi_N(\cdot\,, X)\|_2^2\, dX = \|\psi_N\|_2^2 = 1$$

where we introduced the abbreviation $X = (x_2, \dots, x_N) \in \Omega^{N-1}$.

The one-particle reduced density matrix contains all information of the wave function that is needed to compute the expectation of observables that measure one-particle properties. That is, if $A \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1} \in \mathcal{L}(L^2(\Omega^N))$, then a simple *exercise* shows that

$$\langle \psi_N, A \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1} \psi_N \rangle_{L^2(\Omega^N)} = \operatorname{tr}\big(A\gamma_N^{(1)}\big).$$

If we look for a suitable notion of condensation, then at least (a suitable subclass of) the one-particle observables should be determined by the one-particle wave function that describes the condensate. The notion we consider in this lecture, goes back to a definition proposed by Penrose and Onsager in [52]. Consider a sequence $(\psi_N)_{N\in\mathbb{N}}$ of normalized wave functions in $L^2_s(\Omega^N)$ with associated one-particle reduced density matrices $(\gamma_N^{(1)})_{N\in\mathbb{N}}$ and let $\varphi \in L^2(\Omega)$ be normalized. We say that $(\psi_N)_{N\in\mathbb{N}}$ exhibits complete Bose-Einstein condensation into the wave function $\varphi \in L^2(\Omega)$ if

$$\lim_{N\to\infty} \big\|\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\big\|_{\mathcal{J}_1} = \lim_{N\to\infty} \operatorname{tr}\big|\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\big| = 0 \tag{2.30}$$

This definition is a comparatively strong and an asymptotic notion of condensation. It is an asymptotic definition, because it is a statement about the behaviour of the one-particle reduced densities in the limit $N \to \infty$. It is a strong definition, because it specifies the condensate wave function as well as the asymptotic fraction of particles occupying the condensate. This fraction is given by $\langle \varphi, \gamma_N^{(1)} \varphi\rangle_2$ and (2.30) implies that

$$1 - \langle \varphi, \gamma_N^{(1)} \varphi\rangle_2 = \operatorname{tr}\Big[|\varphi\rangle\langle\varphi|\big(|\varphi\rangle\langle\varphi| - \gamma_N^{(1)}\big)\Big] \le \operatorname{tr}\big|\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\big| \to 0 \quad (N \to \infty).$$

More generally, for every bounded observable $A \in \mathcal{L}(\mathcal{H})$, we have that

$$\big|\operatorname{tr} A\gamma_N^{(1)} - \langle \varphi, A\varphi\rangle\ \big| \le \|A\| \operatorname{tr}\big|\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\big| \to 0 \quad (N \to \infty).$$

That is, all one-body observables are completely determined by the condensate state φ. An important observation is the following equivalent characterization of complete BEC.

Lemma 2.14. *Consider a sequence $(\psi_N)_{N\in\mathbb{N}}$ of normalized wave functions in $L^2_s(\Omega^N)$ with associated one-particle reduced density matrices $(\gamma_N^{(1)})_{N\in\mathbb{N}}$ and let $\varphi \in L^2(\Omega)$ be normalized. Then $(\psi_N)_{N\in\mathbb{N}}$ exhibits complete BEC into φ if and only if*

$$\lim_{N\to\infty} \big(1 - \langle \varphi, \gamma_N^{(1)} \varphi\rangle_2\big) = 0 \tag{2.31}$$

Proof. We claim, first of all, that the compact, self-adjoint operator $\gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \in \mathcal{J}_1$ contains at most one negative eigenvalue[8]. Assume by contradiction that $\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|$ has two negative eigenvalues $\lambda_1, \lambda_2 < 0$ with corresponding orthonormal eigenvectors

[8]This argument goes back to R. Seiringer.

$\xi_1, \xi_2 \in L^2(\Omega)$. Then we can find a linear combination $0 \neq \xi = c_1\xi_1 + c_2\xi_2$, $c_1, c_2 \in \mathbb{C}$, s.t. $c_1\xi_1 + c_2\xi_2$ is orthogonal to φ. This, however, implies that

$$0 \leq \langle \xi, \gamma_N^{(1)} \xi \rangle_2 = \langle c_1\xi_1 + c_2\xi_2, (\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|)(c_1\xi_1 + c_2\xi_2)\rangle_2 = |c_1|^2\lambda_1 + |c_2|^2\lambda_2 < 0$$

Hence, $\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|$ contains at most one negative eigenvalue. Let's denote the eigenvalues of $\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|$ by $(\mu_n)_{n\in\mathbb{N}}$. Since $\operatorname{tr}(\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|) = \sum_{n=1}^\infty \mu_n = 0$, either $\gamma_N^{(1)} - |\varphi\rangle\langle\varphi| = 0$ or we may assume w.l.o.g. that $\mu_1 < 0$ is the only negative eigenvalue of $\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|$. Since $\|\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\|_{\mathcal{L}(\mathcal{H})} = |\mu_1|$, this shows that

$$\begin{aligned} \operatorname{tr}\big|\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\big| = |\mu_1| + \sum_{n=2}^\infty \mu_n = 2\big\|\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\big\|_{\mathcal{L}(\mathcal{H})} \\ \leq 2\big\|\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\big\|_{\mathcal{J}_2} \leq 2^{3/2}\big(1 - \langle\varphi, \gamma_N^{(1)}\varphi\rangle_2\big)^{1/2} \end{aligned} \tag{2.32}$$

where we used that $\|\gamma_N^{(1)}\|_{\mathcal{J}_2} \leq \|\gamma_N^{(1)}\|_{\mathcal{J}_1} = 1$. □

For practical computations, the criterion (2.31) turns out to be quite useful. In the next chapter, we obtain an equivalent formulation of (2.31) in a Fock space setting which underlines very clearly the physical interpretation of the convergence (2.31).

We close this section with a few further remarks on the definition (2.30). As just mentioned, the definition (2.30) implies that, asymptotically, all particles occupy the same one-particle state. Weaker definitions of the concept of Bose-Einstein condensation can be obtained by saying that asymptotically only a finite fraction of size $\lambda \in (0, 1]$ occupies a particular one-particle wave function. An even weaker notion of condensation is the statement that $\liminf_{N\to\infty} \|\gamma_N^{(1)}\|_{\mathcal{L}(\mathcal{H})} > 0$. The original proposal in [52] defines BEC indeed as the property that the largest eigenvalue of the one-particle reduced density operator remains asymptotically of order one.

Finally, we remark that, analogously to the one-particle reduced density matrix, one can define the so called k-particle reduced density matrices, $k = 2, \dots, N$. Given a normalized state $\psi_N \in L^2_s(\Omega^N)$, the k-particle reduced density matrix $\gamma_N^{(k)} \in \mathcal{J}_1(L^2_s(\Omega^k))$ is the positive trace class operator with integral kernel

$$\gamma_N^{(k)}(X_k, Y_k) = \int_{\Omega^{N-k}} \psi_N(X_k, x_{k+1}, \dots, x_N)\overline{\psi}_N(Y_k, x_{k+1}, \dots, x_N)\, dx_{k+1} \dots dx_N,$$

where we abbreviate $X_k = (x_1, \dots, x_k), Y_k = (y_1, \dots, y_k) \in \Omega^k$. One can prove that complete BEC in the sense of (2.30) implies also the convergence

$$\lim_{N\to\infty} \operatorname{tr}\big|\gamma_N^{(k)} - |\varphi^{\otimes k}\rangle\langle\varphi^{\otimes k}|\big| = 0$$

for every fixed $k \in \mathbb{N}$. We refer the interested reader to [32] for a detailed proof.

2.A The Stone-Weierstrass Theorem

To define the continuous functional calculus, we make use of the complex version of the Stone-Weierstrass Theorem as stated and proved in [55, Section IV.3].

Theorem 2.24. *Let X be a compact Hausdorff space and let B be a subalgebra of $C(X;\mathbb{C})$ which is closed under complex conjugation. If B is closed and separates points, meaning that for all $x, y \in X$ there exists some $f \in B$ with $f(x) \neq f(y)$, then $B = C(X;\mathbb{C})$ or for some $x_0 \in X$, we have $B = \{f \in C(X;\mathbb{C}) : f(x_0) = 0\}$. If B separates points and if $\mathbf{1} \in B$, $B = C(X;\mathbb{C})$.*

2.B The Riesz Representation Theorem

We use the following form of the Riesz Representation Theorem characterizing positive linear functionals on $C(X;\mathbb{C})$, the space of continuous, complex-valued functions on a compact metric space X. A careful proof can be found in [66, Section 1.7] (for real-valued continuous functions, but this implies the complex version as well).

Theorem 2.25. *Let X be a compact metric space and let $\phi : C(X;\mathbb{C}) \to \mathbb{C}$ be a positive linear functional such that $\phi(f) \geq 0$ whenever $f \geq 0$ pointwise. Then, there exists a unique finite positive Borel measure $\mu_\phi : \mathcal{B}(X) \to [0,\infty)$ s.t. for all $f \in C(X;\mathbb{C})$ we have*

$$\phi(f) = \int_X f(x)\, d\mu_\phi(x) \tag{2.33}$$

In particular, μ_ϕ inner and outer regular (as it is finite).

Remark 2.5. *It is enough to prove the theorem for real valued continuous functions; this implies the complex valued case as well by splitting a general $f \in C(X;\mathbb{C})$ into its real and imaginary parts. With a little more work (see [66, Chapter 1, Section 7.2]), Theorem 2.25 can be used to show that $\big(C(X;\mathbb{R})\big)^*$ is isometrically isomorphic to the space of finite signed Borel measures, equipped with the total variation norm. Related to this, notice that a positive linear functional $\phi : C(X;\mathbb{C}) \to \mathbb{R}$ is bounded, because*

$$\phi(\|f\|_\infty \pm (f)) \geq 0 \implies |\phi(f)| \leq \phi(1)\|f\|_\infty.$$

Remark 2.6. *The assumption that X is a compact metric space can be relaxed. Another variant of the theorem only assumes e.g. that X is a locally compact Hausdorff space. The version in Theorem 2.25 is sufficient for all applications in these notes.*

Proof. We follow [66, Chapter 1, Section 7.1] and prove the theorem in the setting of real-valued functions. So, let ϕ be a positive linear functional on $C(X;\mathbb{R})$. We first construct a suitable outer measure μ_* on $\mathcal{P}(X)$ with the property that $\mu_*(E_1 \cup E_2) = \mu_*(E_1) + \mu_*(E_2)$ if $\mathrm{dist}(E_1, E_2) > 0$. This yields a regular Borel measure μ_ϕ by Caratheory's construction, see e.g. [65, Chapter 6]. Afterwards we verify the identity (2.33) for μ_ϕ.

To start with the outer measure, we need to relate the measure of a set with the functional ϕ. Heuristically, we would like to define $\mu_*(E) \approx \phi(\chi_E)$ where E denotes the characteristic function on $E \subset X$. Of course, characteristic functions are not in $C(X;\mathbb{R})$, but we can make this idea rigorous through a limiting procedure. We first define

$$\rho(U) = \sup\left\{\phi(f) : \operatorname{supp}(f) \subset U,\, 0 \le f \le 1\right\} \ge 0$$

for $\emptyset \neq U \subset X$ open and $\rho(\emptyset) = 0$. We then set

$$\mu_*(E) = \inf\left\{\rho(U) : E \subset U,\, U \subset X \text{ open}\right\} \ge 0.$$

It is clear that $\mu_*(\emptyset) = 0$ (recall that $\rho(\emptyset) = 0$) and that $\mu_*(E_1) \le \mu_*(E_2)$ if $E_1 \subset E_2$, by definition of μ_*. The sub-additivity of μ_* follows from standard arguments if we prove it first for open sets on which we have $\mu_* = \rho$. So, consider a sequence $(U_k)_{k\in\mathbb{N}}$ of open sets $U_k \subset X$ and set $U = \cup_{k=1}^{\infty} U_k$. Then, if $0 \le f \le 1$ and $\operatorname{supp}(f) \subset U$, then by compactness, we have $\operatorname{supp}(f) \subset \cup_{k=1}^{N} U_k$ for some $N \in \mathbb{N}$. Associated to $(U_k)_{k=1}^{N}$, denote by $(\psi_k)_{k=1}^{N}$ a standard partition of unity, so that in particular $f = \sum_{k=1}^{N} f\psi_k$ with $f\psi_k \in C(X;\mathbb{R})$, $\operatorname{supp}(f\psi_k) \subset U_k$ and $0 \le f\psi_k \le 1$ for each $k = 1, \ldots, N$. Then

$$\phi(f) = \sum_{k=1}^{N} \phi(f\psi_k) \le \sum_{k=1}^{N} \rho(U_k) \le \sum_{k=1}^{\infty} \mu_*(U_k).$$

Taking the supremum over all such f, we conclude that $\mu_*(U) \le \sum_{k=1}^{\infty} \mu_*(U_k)$ as desired. For the general case of sets $(E_k)_{k\in\mathbb{N}}$, pick $\varepsilon > 0$ and choose $(U_k)_{k\in\mathbb{N}}$ so that

$$\mu_*(U_k) \le \mu_*(E_k) + \frac{\varepsilon}{2^k}$$

so that by monotonicity and the previous step

$$\mu_*\left(\bigcup_{k\in\mathbb{N}} E_k\right) \le \sum_{k\in\mathbb{N}} \mu_*(U_k) \le \sum_{k\in\mathbb{N}} \mu_*(E_k) + \varepsilon \sum_{k\in\mathbb{N}} 2^{-k}.$$

Letting $\varepsilon > 0$ tend to zero, we conclude that μ_* is an outer measure.

To see that Caratheodory's construction yields a regular Borel measure, it is enough to prove that

$$\mu_*(E_1 \cup E_2) = \mu_*(E_1) + \mu_*(E_2)$$

whenever $\operatorname{dist}(E_1, E_2) > 0$. Notice that for E_1, E_2 open, this statement is true, by the definition of ρ and the fact that $\operatorname{supp}(f) \subset U_1 \cup U_2$ with $\operatorname{dist}(U_1, U_2) > 0$ if and only if $f = f_1 + f_2$ with $\operatorname{supp}(f_1) \subset U_1, \operatorname{supp}(f_2) \subset U_2$. For the general case, we can choose U_1, U_2 open such that $E_1 \subset U_1, E_2 \subset U_2$ and $\operatorname{dist}(U_1, U_2) > 0$. Then, if $E_1 \cup E_2 \subset U$ for some $U \subset X$ open, we have that

$$\mu_*(U) \ge \mu_*\big((U \cap U_1) \cup (U \cap U_2)\big) = \mu_*(U \cap U_1) + \mu_*(U \cap U_2) \ge \mu_*(E_1) + \mu_*(E_2),$$

which implies that $\mu_*(E_1 \cup E_2) \ge \mu_*(E_1) + \mu_*(E_2)$ by taking the infimum over all open $U \subset X$ open such that $E_1 \cup E_2 \subset U$.

Let us denote from now on by μ_ϕ the finite measure obtained through Caratheodory's construction. It remains to prove the formula (2.33) and to this end, suppose that $f \in C(X;\mathbb{R})$ with $0 \le f \le 1$: the general case can be reduced to this by splitting $g \in C(X;\mathbb{R})$ into the difference of its positive and negative parts and by rescaling. To relate $\phi(f)$ to μ_ϕ, we split f into $N \in \mathbb{N}$ continuous pieces according to the open sets

$$U_n = \{x \in X : f(x) > (n-1)/N\} \subset X.$$

One has $U_{n+1} \subset U_n$ for each n and one can check that $f = \sum_{n=1}^N f_n$, where

$$f_n(x) = \begin{cases} 1/N & : \text{if } x \in U_{n+1} \\ f(x) - (n-1)/N & : \text{if } x \in U_n \cap U_{n+1}^c \\ 0 & : \text{else.} \end{cases}$$

Note that $f_n \in C(X;\mathbb{R})$ with $0 \le f_n \le 1/N$, $\operatorname{supp}(f_n) \subset \overline{U_n} \subset U_{n-1}$. This implies that

$$\mu(U_{n+1}) = \rho(U_{n+1}) \le \phi(Nf_n) = N\phi(f_n) \le N\rho(U_{n-1}) = \mu(U_{n-1}),$$

where the first inequality follows from the fact that $(Nf_n)_{|U_{n+1}} = 1$ and the positivity of the functional ϕ. By linearity, we obtain that

$$\frac{1}{N}\sum_{n=1}^N \mu(U_{n+1}) \le \phi(f) \le \frac{1}{N}\sum_{n=1}^N \mu(U_{n-1}).$$

Similarly, we have that

$$\mu(U_{n+1}) = \int_{U_{n+1}} d\mu_\phi \le N\int_X f_n(x)\,\mu_\phi(dx) \le \mu(U_{n-1}),$$

again by the properties of f_n (and monotonicity of the integral). Thus, we find that

$$\frac{1}{N}\sum_{n=1}^N \mu(U_{n+1}) \le \int_X f(x)\,\mu_\phi(dx) \le \frac{1}{N}\sum_{n=1}^N \mu(U_{n-1})$$

and therefore (recalling $U_{n+1} \subset U_{n-1}$)

$$\left|\phi(f) - \int_X f(x)\,\mu_\phi(dx)\right| \le \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^N \mu(U_{n-1}\cap U_{n+1}^c) \le \frac{2\mu(X)}{N} = 0.$$

Finally, uniqueness follows by approximating $\mu_\phi(U)$ for $U \subset X$ open through

$$\mu_\phi(U) = \lim_{n\to\infty}\phi(f_n)$$

for a suitable sequence $(f_n)_{n\in\mathbb{N}}$ in $C(X;\mathbb{R})$ with $0 \le f_n \le 1$, $\operatorname{supp}(f_n) \subset \overline{U}$ and $\lim_{n\to\infty} f_n(x) = \chi_U(x)$ for all $x \in X$, applying dominated convergence. This implies that ϕ determines μ_ϕ uniquely on open and thus (e.g. by regularity) on Borel sets. □

3 The Bose Gas in the Mean Field Regime

In this section we consider interacting Bose gases in the so called mean field regime. In this regime particles interact through a weak potential which is proportional to the inverse of the number of particles. With such a weak interaction, one expects that the total potential a fixed particle experiences is given by an average or mean field interaction due to the remaining particles. We either consider the particles moving in $\mathbb{R}^3$, trapped in a region of order one by an external potential, or moving in $\mathbb{T}^3 = \mathbb{R}^3/\mathbb{Z}^3$, the three dimensional flat unit torus (that is, the particles are trapped in a box of volume one and we assume periodic boundary conditions). We start our analysis by determining the ground state energy of the interacting Bose gas up to leading order in the limit $N \to \infty$. Moreover, we show that any approximate ground state of the system exhibits complete Bose-Einstein condensation into the minimizer of the non-linear Hartree energy functional. We then go one step further and determine the next to leading order ground state energy as well as the excitation energies, up to errors vanishing in the limit $N \to \infty$. This rigorously establishes the predictions of Bogoliubov theory in the mean field regime.

The study of mean field quantum systems has a long history. There exists a considerable amount of important and interesting literature on the topic. Here, we present only a few selected and simplified results based on the articles [63, 30, 36]. We refer to the lecture notes [54] for a detailed overview of recent developments on the general derivation of Hartree's theory from mean field (and other) systems and for a thorough list of references.

3.1 Ground State Energy and Complete BEC in the Mean Field Regime

In this section we consider N bosons moving in $\mathbb{R}^3$. The Hilbert space describing the system is $L^2_s(\mathbb{R}^{3N})$ and the Hamiltonian H_N^{trap} reads

$$H_N^{\text{trap}} = \sum_{i=1}^N (-\Delta_{x_i} + V_{\text{ext}}(x_i)) + \frac{1}{N} \sum_{1\leq i<j\leq N} v(x_i - x_j) \tag{3.1}$$

We assume $V_{\text{ext}} \in L^\infty_{\text{loc}}(\mathbb{R}^3)$ and s.t. $V_{\text{ext}}(x) \to \infty$ as $|x| \to \infty$. To ignore any regularity issues related to the interaction, we assume for simplicity that $v \in \mathcal{S}(\mathbb{R}^3)$ is a Schwartz function. Moreover, we assume that v is radial and that v has non-negative Fourier transform $\widehat{v} \geq 0$. Under these assumptions H_N^{trap} is essentially self-adjoint on[9] $S_N(C_c^\infty(\mathbb{R}^{3N}))$, by Prop. 2.3. Moreover, by Remark 2.5 and Corollary 2.6, $\sigma(H_N^{\text{trap}}) = \sigma_{\text{d}}(H_N^{\text{trap}})$.

The scaling factor N^{-1} in front of the two-body interaction in (3.1) characterizes the mean field regime. On the one hand, this choice makes the interaction quite weak. In fact, when $N \to \infty$, its strength tends to zero. On the other hand, with such a choice the kinetic and interaction energies can be expected to be of the same order $O(N)$. This means that, although the interaction is quite weak, it can not be neglected, but must have a significant effect on the spectrum and the dynamics of the system.

[9]Here, S_N denotes the symmetrization operator as defined in Section 2.1. Notice that $S_N \in \mathcal{L}(L^2(\mathbb{R}^{3N}))$ is a bounded orthogonal projection and leaves the Hamiltonian H_N invariant.

In the non-interacting case $v = 0$, in the ground state all particles are condensated into the ground state of the one body operator $-\Delta + V_{\text{ext}}$. In particular, all particles are distributed in space independently from one another. If we assume that a weak interaction does not change this picture dramatically, we may hope that the leading order contribution to the ground state energy can still be obtained by minimizing H_N^{trap} over tensor product wave functions. Physically, this means that we expect correlation effects among the particles to be negligible, at least in the context of computing the leading order contribution to the energy. Assuming this for now, we arrive at the prediction that the ground state energy E_N of H_N^{trap} should approximately be equal to

$$E_N \approx N \inf_{\|\varphi\|_2=1} \int dx \, \Big(|\nabla \varphi|^2 + V_{\text{ext}}|\varphi|^2 + \frac{1}{2}\big(v * |\varphi|^2\big)|\varphi|^2 \Big).$$

Before making this statement precise, we first analyze the Hartree energy functional $\mathcal{E}_H^{\text{trap}} : D_H \to \mathbb{R}$, defined on $D_H = H^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3; V_{\text{ext}}(x)\, dx)$ by

$$\mathcal{E}_H^{\text{trap}}(\varphi) = \int dx \, \Big(|\nabla \varphi|^2 + V_{\text{ext}}|\varphi|^2 + \frac{1}{2}\big(v * |\varphi|^2\big)|\varphi|^2 \Big). \tag{3.2}$$

In Theorem 3.1 below we prove the existence and uniqueness of minimizers of $\mathcal{E}_H$. In order to prove the uniqueness statement, we need two technical preparations. We start with the convexity inequality for gradients (see [40, Theorem 7.8]).

Proposition 3.1 (Convexity Inequality for Gradients)**.** *Let $f, g \in H^1(\mathbb{R}^d; \mathbb{R})$. Then*

$$\int \big|\nabla \sqrt{f^2 + g^2}\big|^2(x)\, dx \le \int \big[|\nabla f|^2(x) + |\nabla g|^2(x)\big]\, dx \tag{3.3}$$

If moreover $g > 0$ in the sense that for all compact $K \subset \mathbb{R}^d$ there exists an $\varepsilon > 0$ s.t.

$$\big|\{x \in K : g(x) < \varepsilon\}\big| = 0,$$

then equality holds true in (3.3) *if and only if $f = cg$ for some constant $c \in \mathbb{R}$.*

Proof. First of all, $\sqrt{f^2 + g^2} \in H^1(\mathbb{R}^d)$ (see [40, Theorem 6.17]) with

$$\big(\nabla \sqrt{f^2 + g^2}\big)(x) = \begin{cases} \frac{f\nabla f + g \nabla g}{\sqrt{f^2+g^2}}(x) & \text{if } (f^2+g^2)(x) \neq 0, \\ 0 & \text{else} \end{cases}$$

(3.3) is now a direct consequence of the observation that, for $(f^2 + g^2)(x) \neq 0$, we have

$$\begin{aligned} &|\nabla f|^2(x) + |\nabla g|^2(x) - \big|\nabla \sqrt{f^2+g^2}\big|^2(x) \\ &= |\nabla f|^2(x) + |\nabla g|^2(x) - (f^2+g^2)^{-1}(f^2|\nabla f|^2 + g^2 |\nabla g|^2 + 2fg\nabla f \cdot \nabla g)(x) \\ &= (f^2+g^2)^{-1}(g^2|\nabla f|^2 + f^2|\nabla g|^2 - 2fg\nabla f \cdot \nabla g)(x) = (f^2+g^2)^{-1}|g\nabla f - f\nabla g|^2(x) \ge 0 \end{aligned}$$

Now consider the case of equality in (3.3). From the last identity, we see that this implies $(g\nabla f)(x) = (f \nabla g)(x)$ for *a.e.* $x \in \mathbb{R}^d$. We will use this fact to show that $f/g \in L^1_{\text{loc}}(\mathbb{R}^d)$

has vanishing distributional derivative which implies $f = cg$. To this end, consider an arbitrary $\varphi \in C_c^\infty(\mathbb{R}^d)$, then $\varphi/g \in H^1(\mathbb{R}^d)$ with

$$\nabla(\varphi/g) = \nabla\varphi/g - \varphi\nabla g/g^2.$$

This implies

$$\int (f/g)\nabla\varphi = \int f\nabla(\varphi/g) + \int f\varphi\nabla g/g^2 = -\int (\varphi/g)\nabla f + \int (\varphi/g^2)g\nabla f = 0$$

by integration by parts in $H^1(\mathbb{R}^d)$. We conclude that $\nabla(f/g) = 0$ in $\mathcal{D}'(\mathbb{R}^d)$. □

When proving the uniqueness of the minimizer for the Hartree function $\mathcal{E}_H$, we need to apply the statement about equality in (3.3). To be able to apply it, we need in addition the following result which provides a lower bound on eigenfunctions of Schrödinger operators. The following proposition is adapted from [40, Theorems 9.9 and 9.10].

Proposition 3.2. *Let $\Omega \subset \mathbb{R}^d$ be open and connected, let $f \in C(\Omega, [0,\infty))$ be non-negative and let $W \in L^\infty_{loc}(\Omega)$. Assume that f satisfies in distributional sense*

$$-\Delta f + Wf \geq 0. \tag{3.4}$$

Then, for each compact set $K \subset \Omega$, there exists a constant $C > 0$, which is independent of f, such that

$$f(x) \geq C \int_K f(y)\, dy, \qquad \forall x \in K \tag{3.5}$$

Proof. Let K be compact, $R > 0$ and assume that $N \in \mathbb{N}$ balls $B_i = B_R(x_i)$, where $x_i \in K$ for $i = 1, \dots, N$, cover K. We define $F_i = \int_{B_i} f(y)\, dy$ and since

$$\int_K f(x)\, dx \leq \sum_{i=1}^N \int_{B_i} f(y)\, dy \leq N \max_{i=1,\dots,N} F_i$$

we may assume w.l.o.g. that $F_1 \geq N^{-1} \int_K f(y)\, dy$. We then claim that there exists some $0 < \delta < 1$ s.t. for each $i = 1, \dots, N$, we have

$$f(w) \geq \delta F_i = \delta \int_{B_i} f(y)\, dy, \qquad \forall w \in B_i \tag{3.6}$$

Assuming this for the moment, let $x \in K$ and let $\gamma \in C([0,1], \mathbb{R}^d)$ be a continuous curve that connects x with $x_1 \in B_1$. We can cover its trace by finitely many balls $B_{j_1}, B_{j_2}, \dots, B_{j_M}$, $M \leq N$, with the property that $B_{j_k} \cap B_{j_{k+1}} \neq \emptyset$. (3.6) implies

$$F_{j_{k+1}} \geq \int_{B_{j_k} \cap B_{j_{k+1}}} f(y)\, dy \geq \delta \big|B_{j_k} \cap B_{j_{k+1}}\big| F_{j_k}.$$

Defining $\alpha = \min\big(1/2, \min\big\{\big|B_i \cap B_j\big| : B_i \cap B_j \neq \emptyset\big\}\big)$, we conclude

$$F_{j_{k+1}} \geq \delta\alpha F_{j_k}$$

Using again (3.6) and iterating the previous bound until we arrive at $F_1 \ni x_1$, we conclude that we have

$$f(x) \geq \delta(\delta\alpha)^{M-1} F_1 \geq N^{-1}\delta(\delta\alpha)^{M-1} \int_K f(y)\, dy$$

Since $x \in K$ was arbitrary, this proves the claim with $C = N^{-1}\delta(\delta\alpha)^{N-1}$. Notice that C depends on K, but it is independent of f.

It remains to prove (3.6). To this end, let $\Omega' \subset\subset \Omega \subset \mathbb{R}^d$ be open and such that

$$\bigcup_{i=1}^{N} B_{3R}(x_i) \subset \Omega'.$$

Moreover, let $\mu > 0$ be s.t. $W_{|\Omega'} \leq \mu^2$. As a consequence, the restriction of f to Ω', that is $g = f_{|\Omega'} \in C(\Omega', [0, \infty))$, satisfies in distributional sense

$$(-\Delta + \mu^2)g \geq 0. \tag{3.7}$$

The lower bound on g is based on a comparison argument between g and the positive, radially symmetric solution $J \in C^\infty(\mathbb{R}^d, (0; \infty))$ of

$$(-\Delta + \mu^2)J = 0$$

with initial condition $J(0) = 1$. Such solutions exist and they can be expressed explicitly in terms of Bessel functions. We use this here as a fact and refer the interested reader to [40, Theorem 9.9] for more details about this. In the special case $\Omega = \mathbb{R}^3$, which is the only relevant case for us in these notes, one has

$$J(x) = \frac{\sinh(\mu|x|)}{\mu|x|}$$

for all $x \in \mathbb{R}^3$. Below, we denote by $J(r)$ for $r > 0$ the value $J(x)$ for some (and hence, by radial symmetry, for all) $x \in \mathbb{R}^d$ with $|x| = r$.

Now, let us prove (3.6). Assume first that $g \in C^\infty(\mathbb{R}^d)$. In this case (3.7) holds pointwise. Let $z \in \mathbb{R}^d$ be arbitrary and define $J_z \in C^\infty(\mathbb{R}^d, (0, \infty))$ as the translation

$$J_z(x) = J(x - z).$$

Then, by (3.7), the radial symmetry of J and integration by parts, we get

$$\begin{aligned} 0 &\geq \frac{1}{|S_r(0)|} \int_{B_r(z)} \big[J_z(\Delta g) - g(\Delta J_z)\big](x)\, dx = \frac{1}{|S_r(0)|} \int_{B_r(z)} \nabla \cdot (J_z \nabla g - g \nabla J_z)(x)\, dx \\ &= \frac{1}{|S_r(0)|} \int_{S_r(z)} (J_z \nabla g - g \nabla J_z) \cdot d\mathbf{S} = J(r)\partial_r [g]_{z,r}(r) - [g]_{z,r}(r)(\partial_r J)(r) \end{aligned}$$

for all $r > 0$. Here, $[g]_{z,r}$ denotes the spherical average of g over $S_r(z)$, recalling that

$$\int_{S_r(z)} (\nabla f) \cdot d\mathbf{S} = \int_{S_r(0)} (\nabla f)(\omega + z) \cdot \frac{\omega}{|\omega|} dS(\omega) = r^{d-1} \int_{S_1(0)} \partial_r f(r\omega + z)\, dS(\omega).$$

The above arguments show that

$$\partial_r \frac{[g]_{z,\cdot}}{J} = \frac{J(\partial_r [g]_{z,\cdot}) - (\partial_r J)[g]_{z,\cdot}}{J^2} \leq 0,$$

so that the map $r \mapsto [g]_{z,r}/J(r)$ is decreasing. By continuity of g, $J(0) = 1$ and

$$\lim_{r \to 0} [g]_{z,r} = \lim_{r \to 0} \frac{1}{|S_1(0)|} \int_{S_1(z)} dS(\omega)\, g(z + r\omega) = g(z),$$

we arrive at

$$g(z) \geq \frac{[g]_{z,r}}{J(r)}$$

for all $r > 0$ and $z \in \Omega$. Integrating the last bound implies for all $w \in B_i \big(= B_R(x_i)\big)$

$$\begin{aligned} g(w) &\geq \frac{1}{|B_{2R}(0)|} \int_0^{2R} dr\, r^{d-1} \frac{|S_1(0)| [g]_{w,r}}{J(r)} \\ &\geq C_{2R} \int_{B_{2R}(w)} g(y)\, dy \geq C_{2R} \int_{B_R(x_i)} g(y)\, dy = C_{2R} \int_{B_i} f(y)\, dy \end{aligned} \tag{3.8}$$

for $C_{2R} = \big(|B_{2R}(0)| \sup_{y \in B_{2R}(0)} J(y)\big)^{-1}$. Choosing $\delta = \min(1/2, C_{2R}) \in (0,1)$ proves (3.6) for $g \in C^\infty(\Omega')$, recalling that $g = f_{|\Omega'}$. Finally, for a general $g \in C(\Omega')$, we use a mollifying sequence and prove the pointwise lower bound (3.8) first for *a.e.* $w \in B_i$. Since g is continuous and the lower bound on the right hand side in (3.8) is independent of $w \in B_i$, (3.8) holds true for all $w \in B_R(z)$. □

Theorem 3.1. *The Hartree energy functional* (3.2) *admits a pointwise positive minimizer* $\varphi_H \in D_H \cap \{\psi \in L^2(\mathbb{R}^3) : \|\psi\|_2 = 1\}$ *which is unique up to a constant phase and which satisfies the Euler-Lagrange equation*

$$\big(-\Delta + V_{\text{ext}} + v * |\varphi_H|^2 \big) \varphi_H = \epsilon_0\, \varphi_H \tag{3.9}$$

in $\mathcal{D}'$, *where*

$$\epsilon_0 = \mathcal{E}_H^{\text{trap}}(\varphi_H) + \frac{1}{2} \big\langle \varphi_H, \big(v * |\varphi_H|^2\big) \varphi_H \big\rangle = e_{\text{H}} + \frac{1}{2} \big\langle \varphi_H, \big(v * |\varphi_H|^2\big) \varphi_H \big\rangle. \tag{3.10}$$

Moreover, φ_H *decays exponentially at infinity and* $\varphi_H \in C^1(\mathbb{R}^3)$.

Proof. The existence of a minimizer follows from the direct methods of the calculus of variations. For the remaining claims, we argue as in [45, Appendix A].

We start with a minimizing sequence $(\varphi_j)_{j \in \mathbb{N}}$ in D_H, $\|\varphi_j\|_2 = 1 \,\forall\, j \in \mathbb{N}$, and observe that $\sup_{j \in \mathbb{N}} \|\phi_j\|_{H^1} \leq C$ for some $C > 0$. Here, we make use of the fact that V_{ext} is bounded from below which follows from our assumptions. Hence, we find a weakly converging subsequence in $H^1(\mathbb{R}^3)$, denoted for simplicity again by $(\varphi_j)_{j \in \mathbb{N}}$. Denote by $\varphi \in H^1(\mathbb{R}^3)$ the weak limit. Since the sequence is minimizing for $\mathcal{E}_H^{\text{trap}}$, we may assume

$$\sup_{j \in \mathbb{N}} \int V_{\text{ext}} |\varphi_j|^2 < \infty.$$

Using the last bound and that $V_{\rm ext}(x) \to \infty$ as $|x| \to \infty$, we find for suitable $R, R' > 0$

$$\sup_{j\in\mathbb{N}} \int_{B_R(0)^C} |\varphi_j(x)|^2 \, dx \le \frac{1}{R'} \sup_{j\in\mathbb{N}} \int_{V_{\rm ext}\ge R'} V_{\rm ext}(x)|\varphi_j(x)|^2 \, dx \to 0 \quad (R \to \infty)$$

Using the compactness of $H^1(B_R(0)) \hookrightarrow L^2(B_R(0))$, we may assume w.l.o.g. that the sequence $((\varphi_j)_{|B_R(0)})_{j\in\mathbb{N}}$ converges strongly in $L^2(B_R(0))$ to $\varphi_{|B_R(0)}$. Choosing R large enough, this implies that $\|\varphi\|_2 \ge 1 - \varepsilon$, for a given $\varepsilon > 0$. Since the L^2-norm is weakly sequentially lower semi-continuous, we also have that $\|\varphi\|_2 \le 1$ so that $\|\varphi\|_2 = 1$. Choosing another subsequence if necessary, we may therefore assume that $(\varphi_j)_{j\in\mathbb{N}}$ converges to φ in $L^2(\mathbb{R}^3)$ and for *a.e.* $x \in \mathbb{R}^3$ (here, we use the fact that in Hilbert spaces weak convergence and convergence of the norm implies norm convergence).

If $V_{\rm ext}\chi_{\mathbb{R}^3\setminus B_R(0)} \ge 0$ and $|V_{\rm ext}|\chi_{B_R(0)} \le C$, the L^2-convergence, the pointwise convergence and Fatou's lemma imply

$$\begin{aligned}
&\liminf_{j\to\infty} \int dx \, \big(V_{\rm ext}|\varphi_j|^2 + \frac{1}{2}\big(v * |\varphi_j|^2\big)|\varphi_j|^2\big) \\
&\ge \int_{\mathbb{R}^3\setminus B_R(0)} dx \, V_{\rm ext}|\varphi|^2 + \lim_{j\to\infty} \int_{B_R(0)} dx \, V_{\rm ext}|\varphi_j|^2 + \frac{1}{2} \int dx \, \big(v * |\varphi|^2\big)|\varphi|^2 \\
&= \int dx \, \big(V_{\rm ext}|\varphi|^2 + \frac{1}{2}\big(v * |\varphi|^2\big)|\varphi|^2\big).
\end{aligned}$$

Since the H^1-norm is also weakly sequentially lower semicontinuous (and $\|\varphi_j\|_2 = 1$ for every $j \in \mathbb{N}$), we conclude that $\varphi \in D_H$ is a normalized minimizer of $\mathcal{E}_H^{\rm trap}$, because

$$\inf_{\psi\in D_H, \|\psi\|_2=1} \mathcal{E}_H^{\rm trap}(\psi) = \liminf_{j\to\infty} \mathcal{E}_H^{\rm trap}(\varphi_j) \ge \mathcal{E}_H^{\rm trap}(\varphi).$$

The fact that φ satisfies the Euler-Lagrange equation (3.9) follows from differentiating the continuously differentiable map $t \mapsto \mathcal{E}_H^{\rm trap}(\varphi_{\psi,t})$, where $\varphi_{\psi,t} = \frac{\varphi + t\psi}{\|\varphi+t\psi\|_2}$ and where $\psi \in C_c^\infty(\mathbb{R}^3)$, at its minimum $t = 0$.

Next, let us prove that the minimizer is unique, up to multiplication by a constant. Using Corollary 2.7 and Proposition 3.1, we first show that any minimizer is pointwise positive after multiplication by a constant phase. In fact, the inequality

$$\int \big|\nabla|\varphi(x)|\big|^2 \, dx \le \int |\nabla\varphi(x)|^2 \, dx$$

implies that $\mathcal{E}_H^{\rm trap}(|\varphi|) \le \mathcal{E}_H^{\rm trap}(\varphi)$. Hence, if φ is a minimizer, also $|\varphi|$ is a minimizer and therefore satisfies the Euler-Lagrange equation (3.9). But this implies that $|\varphi|$ must be equal to the unique, positive ground state wave function of $-\Delta + W$ where $W = V_{\rm ext} + v * |\varphi|^2 \in L^\infty_{\rm loc}(\mathbb{R}^3)$. If it was not the ground state wave function, $|\varphi|$ would be an eigenfunction[10] orthogonal to the positive ground state of $-\Delta + W$. But $|\varphi|$ is

[10]Notice that $D(-\Delta+W) = D(-\Delta+V_{\rm ext})$, because $v*|\varphi|^2$ is a bounded perturbation. Since $-\Delta+V_{\rm ext}$ is essentially self-adjoint on $\mathcal{D}$, the Euler-Lagrange equation (3.9) implies that $|\varphi| \in D(-\Delta + W)$.

non-negative and normalized, so it can not be orthogonal to a strictly positive function. Since φ also satisfies the Euler-Lagrange equation (3.9), it follows that φ must also be a ground state wave function of $-\Delta + W$. Hence, by Corollary 2.7, φ is equal to $|\varphi|$, up to mulitplication by a constant of modulus one.

Let us remark that $|\varphi|$ is in fact positive in the sense of Proposition 3.1. For elliptic regularity and the Euler-Lagrange equation (3.9) imply that $|\varphi|$ has a continuous representative (see [40, Theorem 10.2]). Thus, we can apply Proposition 3.2 which shows that $|\varphi|$ is positive in the sense of Proposition 3.1.

Now, to prove the uniqueness of the minimizer, let's assume we are given two pointwise positive minimizers $\sqrt{\rho_1}, \sqrt{\rho_2} \in D_H$ with $\|\sqrt{\rho_i}\|_2 = 1$ for $i = 1, 2$. Then also $\Phi_{1/2} = \left(\frac{1}{2}\rho_1 + \frac{1}{2}\rho_2\right)^{1/2} \in D_H$ with $\|\Phi_{1/2}\|_2 = 1$. If we can show that the map $\rho \mapsto \mathcal{E}_H^{\text{trap}}(\sqrt{\rho})$ is strictly convex for positive $\rho > 0$ with $\|\rho\|_1 = 1$, we deduce from

$$\inf_{\psi \in D_H, \|\psi\|_2 = 1} \mathcal{E}_H^{\text{trap}}(\psi) \leq \mathcal{E}_H^{\text{trap}}(\Phi_{1/2}) \leq \frac{1}{2}\mathcal{E}_H^{\text{trap}}(\rho_1) + \frac{1}{2}\mathcal{E}_H^{\text{trap}}(\rho_2) = \inf_{\psi \in D_H, \|\psi\|_2 = 1} \mathcal{E}_H^{\text{trap}}(\psi),$$

that $\sqrt{\rho_1} = \sqrt{\rho_2}$, that is, uniqueness of the minimizer of $\mathcal{E}_H^{\text{trap}}$. To prove the convexity, define for $t \in (0, 1)$ the function Φ_t by $\Phi_t = \left(t\rho_1 + (1 - t)\rho_2\right)^{1/2}$. We then have trivially

$$\int V_{\text{ext}}(x)\Phi_t^2(x)\, dx = t \int V_{\text{ext}}(x)\rho_1(x)\, dx + (1 - t) \int V_{\text{ext}}\rho_2(x)\, dx.$$

By $\widehat{v} \geq 0$ and the convexity of $y \mapsto y^2$, we also find

$$\begin{aligned}\left\langle \Phi_t^2, v * \Phi_t^2 \right\rangle &= \left\langle v, \Phi_t^2(-.) * \Phi_t^2 \right\rangle = \left\langle \widehat{v}, |\widehat{(\Phi_t^2)}|^2 \right\rangle \\ &\leq t\left\langle \widehat{v}, |\widehat{\rho_1}|^2 \right\rangle + (1 - t)\left\langle \widehat{v}, |\widehat{\rho_2}|^2 \right\rangle = t\left\langle \rho_1, v * \rho_1 \right\rangle + (1 - t)\left\langle \rho_2, v * \rho_2 \right\rangle\end{aligned}$$

for smooth compactly supported functions ρ_1, ρ_2. By density of $C_c^\infty(\mathbb{R}^3)$ in $L^1(\mathbb{R}^3)$, we conclude the convexity of the interaction term on all of $L^1(\mathbb{R}^3)$. Finally, the map $\rho \mapsto \int |\nabla\sqrt{\rho}|^2$ is convex by Proposition 3.1 which implies that

$$\int |\nabla\sqrt{t\rho_1 + (1 - t)\rho_2}|^2 \leq t \int |\nabla\sqrt{\rho_1}|^2 + (1 - t) \int |\nabla\sqrt{\rho_2}|^2.$$

On the set of strictly positive $\rho > 0$ with $\|\rho\|_1 = 1$, it is strictly convex, because in this set equality in Proposition 3.1 holds true if and only if $\rho_1 = c\rho_2$ for some $c > 0$. The normalization $\|\rho_1\|_1 = \|\rho_2\|_1 = 1$ implies $c = 1$ so that $\rho_1 = \rho_2$, proving uniqueness.

From now on, we denote by φ_H the unique, positive and normalized minimizer of $\mathcal{E}_H^{\text{trap}}$ in D_H. It remains to show that φ_H has exponential decay at infinity. Once this is proved, the Euler-Lagrange equation (3.9) implies that $\Delta\varphi_H \in L^\infty_{\text{loc}}(\mathbb{R}^3)$, which in turn implies $\varphi_H \in C^1(\mathbb{R}^3)$ (see [40, Theorem 10.2]).

To prove the exponential decay, fix some $t > 0$ so that

$$(-\Delta + t^2)\varphi_H = -(W - \varepsilon_0 - t^2)\,\varphi_H$$

where $W = V_{\text{ext}} + (v * |\varphi|^2) \in L^\infty_{\text{loc}}(\mathbb{R}^3)$. This equality holds true in $\mathcal{D}'$. Recalling that $W(x) \to \infty$ as $|x| \to \infty$, it follows that in $\mathcal{D}'$ we have

$$(-\Delta + t^2)\varphi_H \leq -\chi_{B_R(0)}(W - \epsilon_0 - t^2)\,\varphi_H$$

for some sufficiently large $R > 0$ and, by continuity, this inequality remains true in $\mathcal{S}'$.

Now, for $t > 0$, the operator $(-\Delta + t^2)$ has a bounded inverse whose integral kernel is given by the Yukawa-potential Y_t (see [40, Theorem 6.23]), defined pointwise by

$$Y_t(x) = (4\pi|x|)^{-1}\exp(-t|x|)$$

for $x \in \mathbb{R}^3$. Moreover, $(-\Delta + t^2)$ and its inverse leave $\mathcal{S}$ invariant (*why?*) which implies

$$0 < \varphi_H(x) \leq -\int_{B_R(0)} Y_t(x-y)(W(y) - \varepsilon_0 - t^2)\varphi_H(y)\,dy$$

for *a.e.* $x \in \mathbb{R}^3$. The r.h.s. of the last equation can be estimated by

$$\begin{aligned}
&\sup_{x\in\mathbb{R}^3}\Big[-\exp(|x|t)\int_{B_R(0)} Y_t(x-y)(W(y) - \varepsilon_0 - t^2)\varphi_H(y)\,dy\Big]\\
&= \sup_{x\in\mathbb{R}^3}\Big[-\int_{B_R(0)} \frac{\exp((|x|-|x-y|)t)}{4\pi|x-y|}(W(y) - \varepsilon_0 - t^2)\varphi_H(y)\,dy\Big]\\
&\leq C_{R,t,\epsilon_0}\sup_{x\in\mathbb{R}^3}\Big[\int_{B_R(0)} \frac{\exp(2Rt)}{4\pi|x-y|^2}\,dy\Big]^{1/2}\Big[\int_{B_R(0)} \varphi_H^2(y)\,dy\Big]^{1/2} \leq C < \infty
\end{aligned}$$

for some constant $C > 0$, which is independent of $x \in \mathbb{R}^3$. In the last step, we have used that $W \in L^\infty_{\text{loc}}(\mathbb{R}^3)$. Hence, $0 < \varphi_H(x) \leq C\exp(-|x|t)$ for *a.e.* $x \in \mathbb{R}^3$. □

Problem 3.1. *Show that $(-\Delta + t^2)^{-1}$ acts as convolution with Y_t, defined by*

$$x \mapsto Y_t(x) = (4\pi|x|)^{-1}\exp(-t|x|).$$

Problem 3.2. *Let $\Omega \subset \mathbb{R}^n, n \geq 3$, be open and bounded with $\partial\Omega$ of class C^1. Let $p > 2$ and assume that $f \in L^2(\Omega)$. Show that, in the sense of distributions, there exists a solution $u \in H^1_0(\Omega)$ to the boundary value problem*

$$\begin{cases} -\Delta u + |u|^{p-2}u = f & \text{in } \Omega,\\ u_{|\partial\Omega} = 0. \end{cases}$$

Having established the existence and uniqueness of the minimizer of $\mathcal{E}_H^{\text{trap}}$, the rest of this section is devoted to the proof of the following theorem about mean field systems.

Theorem 3.2 (Ground State Energy and BEC)**.** *Let $(\psi_N)_{N\in\mathbb{N}}$, $\|\psi_N\|_2 = 1\ \forall\ N \in \mathbb{N}$, be a sequence of wave functions in the domain of H_N^{trap} defined in* (3.1)*, such that there exists a constant $\zeta > 0$ so that for all $N \in \mathbb{N}$*

$$\langle\psi_N, H_N^{\text{trap}}\psi_N\rangle \leq Ne_H + \zeta.$$

Then $(\psi_N)_{N\in\mathbb{N}}$ exhibits complete BEC into the minimizer $\varphi_H \in D_H$ of $\mathcal{E}_H^{\text{trap}}$.

More precisely, denoting by $(\gamma_N^{(1)})_{N\in\mathbb{N}}$ the one-particle reduced density matrices of $(\psi_N)_{N\in\mathbb{N}}$, there exists a constant $C > 0$, independent of $N \in \mathbb{N}$ and $\zeta > 0$, such that

$$1 - \langle \varphi_H, \gamma_N^{(1)} \varphi_H \rangle \leq C(1+\zeta)N^{-1}. \tag{3.11}$$

Moreover, the ground state E_N of H_N^{trap} satisfies

$$E_N = Ne_H + O(1). \tag{3.12}$$

Remarks:

1) Equation (3.12) of Theorem 3.2 implies in particular that every ground state of H_N^{trap} exhibits complete BEC into the minimizer φ_H of the Hartree functional $\mathcal{E}_H^{\text{trap}}$.

2) In view of the ground state energy asymptotics (3.12), we call a sequence $(\psi_N)_{N\in\mathbb{N}}$ of normalized wave functions with the property that $\langle \psi_N, H_N^{\text{trap}} \psi_N \rangle \leq Ne_H + \zeta$ a sequence of approximate ground state wave functions.

3) It is clear that the threshold $\zeta > 0$ on the energy may depend on $N \in \mathbb{N}$, that is, $\zeta = \zeta(N)$. As long as $\zeta(N) = o(N)$, the bound (3.11) implies complete BEC.

4) The rate of the condensate depletion of order $O(N^{-1})$ in (3.11) is optimal. This can be proved, for example, with the methods explained in the next Section 3.2.

5) The validity of Hartree's approximation $E_N = Ne_H + o(N)$ is valid under much less restrictive assumptions, compared to those of this section. In particular, the assumption $\widehat{v} \geq 0$ is not needed. We refer the interested reader to [34, 35, 54].

Proof. The proof follows [63, 30]. Using the positive definiteness of the interaction v, we give a lower bound on the many body interaction in terms of the Hartree interaction energy. The lower bound implies complete BEC into φ_H and that $E_N \geq Ne_H + O(1)$. The upper bound on E_N follows by using a simple trial state (a product wave function).

Before we bound the many body interaction from below, let us notice that the Min-Max Principle 2.17 and its Corollary 2.6 imply that the one body operator

$$\mathbf{h} = -\Delta + V_{\text{ext}} + (v * \varphi_H^2)$$

has purely discrete spectrum $\sigma(\mathbf{h}) = \{\epsilon_j \in \mathbb{R} : j \in \mathbb{N}\} = \sigma_{\text{d}}(\mathbf{h})$ with the ground state energy ϵ_0 defined in (3.10). We may order the eigenvalues s.t. $\epsilon_0 < \epsilon_1 \leq \epsilon_2 \leq \ldots$ where the strict inequality $\epsilon_0 < \epsilon_1$ follows from the uniqueness of the ground state φ_H of $\mathbf{h}$. In the following let's denote by $\{\varphi_j \in L^2(\mathbb{R}^3) : j \in \mathbb{N}\}$, $\varphi_0 = \varphi_H$, a complete orthonormal eigenbasis of $\mathbf{h}$ such that $\mathbf{h}\varphi_j = \epsilon_j \varphi_j$ for all $j \in \mathbb{N}$.

With these preliminary observations, we start to prove the lower bound on E_N. To get the right lower bound, it is natural to try to compare H_N^{trap} with a non-interacting

Hamiltonian whose ground state vector is $\varphi_0^{\otimes N}$ and whose ground state energy is given to leading order by Ne_H. Such an efffective Hamiltonian is given by

$$H_N^{\mathrm{eff}} = \sum_{j=1}^N \Big(\mathbf{h}_{x_j} - \frac{1}{2}\big\langle \varphi_H, \big(v * |\varphi_H|^2\big)\varphi_H\big\rangle\Big) = Ne_H + \sum_{j=1}^N \big(\mathbf{h}_{x_j} - \epsilon_0\big),$$

recalling the Euler-Lagrange equation solved by φ_0. Now notice that the potential energy can be written as

$$\frac{1}{N}\sum_{1\le x_i<x_j\le N} v(x_i-x_j) \approx \frac{1}{2N}\int dxdy\, v(x-y)\Big(\sum_{i=1}^N \delta(x-x_i)\Big)\Big(\sum_{j=1}^N \delta(y-x_j)\Big)$$

and, similarly, that the mean field interaction contribution to H_N^{eff} can be written as

$$\sum_{j=1}^N (v*\varphi_0^2)(x_j) = \int dxdy\,\Big(\sum_{j=1}^N \delta(x-x_j)\Big)v(x-y)\varphi_0^2(y).$$

To connect the two expressions, we can use the positive definiteness of v and complete the square to obtain a lower bound on the total potential energy:

$$\begin{aligned} 0 &\le \int \Big(\varphi_0^2(x) - \frac{1}{N}\sum_{i=1}^N \delta(x-x_i)\Big)v(x-y)\Big(\varphi_0^2(y) - \frac{1}{N}\sum_{j=1}^N \delta(y-x_i)\Big)\,dxdy \\ &= \langle \varphi_0^2, v*\varphi_0^2\rangle - \frac{2}{N}\sum_{i=1}^N (v*\varphi_0^2)(x_i) + \frac{2}{N^2}\sum_{1\le i<j\le N} v(x_i-x_j) + \frac{1}{N}v(0). \end{aligned}$$

This implies

$$\begin{aligned} \frac{1}{N}\sum_{1\le i<j\le N} v(x_i-x_j) &\ge \sum_{i=1}^N (v*\varphi_0^2)(x_i) - \frac{N}{2}\langle \varphi_0^2, v*\varphi_0^2\rangle - \frac{1}{2}v(0) \\ &\ge \sum_{i=1}^N (v*\varphi_0^2)(x_i) - \frac{N}{2}\langle \varphi_0^2, v*\varphi_0^2\rangle + O(1). \end{aligned} \tag{3.13}$$

To make the argument rigorous, we replace the δ-functions by smooth $(f_\epsilon)_{\epsilon>0}$, $f_\epsilon(x) = \epsilon^{-3}f(x/\epsilon)\,\forall x\in\mathbb{R}^3$, for some radial $0\le f\in C_c^\infty(\mathbb{R}^3)$ with $\int_{\mathbb{R}^3} f(x)\,dx = 1$ and use that

$$\begin{aligned} 0 &\le \lim_{\epsilon\to 0}\int \Big(\varphi_0^2(x) - \frac{1}{N}\sum_{i=1}^N f_\epsilon(x-x_i)\Big)v(x-y)\Big(\varphi_0^2(y) - \frac{1}{N}\sum_{j=1}^N f_\epsilon(y-x_i)\Big)\,dxdy \\ &= \int \Big(\varphi_0^2(x) - \frac{1}{N}\sum_{i=1}^N \delta(x-x_i)\Big)v(x-y)\Big(\varphi_0^2(y) - \frac{1}{N}\sum_{j=1}^N \delta(y-x_i)\Big)\,dxdy. \end{aligned}$$

The lower bound (3.13) implies

$$H_N^{\rm trap} \geq Ne_H + \sum_{i=1}^N (\mathbf{h}_{x_i} - \epsilon_0) + O(1) = H_N^{\rm eff} + O(1).$$

Now, notice that in $L^2(\mathbb{R}^3)$ we have the operator inequalities

$$\mathbf{h} - \epsilon_0 = \sum_{j=0}^\infty \epsilon_j |\varphi_j\rangle\langle\varphi_j| - \epsilon_0 = \sum_{j=1}^\infty (\epsilon_j - \epsilon_0)|\varphi_j\rangle\langle\varphi_j| \geq (\epsilon_1 - \epsilon_0)\big(1 - |\varphi_0\rangle\langle\varphi_0|\big) \geq 0.$$

Hence, we have for any normalized $\psi_N \in D(H_N^{\rm trap})$ the lower bound

$$\langle \psi_N H_N^{\rm trap} \psi_N\rangle \geq Ne_H + N(\epsilon_1 - \epsilon_0)\big(1 - \langle \varphi_0, \gamma_N^{(1)}\varphi_0\rangle\big) + O(1).$$

If we assume to have an approximate ground state, that is $\langle \psi_N, H_N^{\rm trap}\psi_N\rangle \leq Ne_H + \zeta$, we obtain (3.11). To prove (3.12), we use that $1 - |\varphi_H\rangle\langle\varphi_H| \geq 0$ and obtain

$$Ne_H + O(1) \leq E_N = \inf_{\substack{\psi_N \in D(H_N^{\rm trap}),\\ \|\psi_N\|_2 = 1}} \langle \psi_N, H_N^{\rm trap}\psi_N\rangle \leq \langle \varphi_0^{\otimes N}, H_N^{\rm trap}\varphi_0^{\otimes N}\rangle = Ne_H.$$

This shows that $E_N = Ne_H + O(1)$. □

3.2 Excitation Spectrum of Bose Gases in the Mean Field Regime

In the previous section, we saw that the leading order term of the ground state energy of a mean field Hamiltonian of the form (3.1) is given by the minimum of the Hartree functional, defined in (3.2): Theorem 3.2 shows that

$$E_N = Ne_H + O(1)$$

and that any approximate ground state exhibits complete BEC into the minimizer $\varphi_{\rm H}$ of the Hartree energy functional. A more ambitious question is to ask whether we can find an explicit expression for the contribution $O(1)$ in Theorem 3.2, valid up to errors that vanish in the limit $N \to \infty$. Moreover, we may also ask for an approximation of the eigenvalues lying above E_N (the excitation spectrum) and, moreover, for an approximation of the ground state wave function in $L^2_s(\mathbb{R}^{3N})$ (and not only in the trace class sense). The rigorous derivation of these approximations is the goal of this section.

We work in this section in $L^2_s(\Lambda^N)$, where $\Lambda = \mathbb{T}^3 = \mathbb{R}^3/\mathbb{Z}^3$ denotes the three dimensional unit torus. The Hamiltonian H_N of the system is given by

$$H_N = \sum_{i=1}^N (-\Delta_{x_i}) + \frac{1}{N}\sum_{1\leq i<j\leq N} v(x_i - x_j). \tag{3.14}$$

We assume that $v \in C_c^\infty\big((-\frac{1}{2},\frac{1}{2})^3\big)$ is radially symmetric and such that $\widehat{v}(p) \geq 0$ for all $p \in \Lambda^* = 2\pi\mathbb{Z}^3$. Note that, by slight abuse of notation, we identify v in the following with its periodic extension to a function in $C^\infty(\mathbb{T}^3)$ (similarly, in (3.14) the difference $x_i - x_j$ denotes the distance on the unit torus).

Observe that H_N is self-adjoint in $H_s^2(\Lambda^N)$, which follows from Theorem 2.4 and Theorem 2.21. Notice, moreover, that the spectrum of H_N equals $\sigma(H_N) = \sigma_{\mathrm{d}}(H_N)$ by the Min-Max Theorem 2.17 and the fact that $H_N \geq \sum_{i=1}^N (-\Delta_{x_i})$. On the domain

$$D_H = \Big\{ \varphi \in L^2(\Lambda) : \sum_{p\in\Lambda^*} |p|^2 |\widehat{\varphi}_p|^2 < \infty \Big\} \, (= H^1(\Lambda)),$$

we define $\mathcal{E}_H : D_H \to \mathbb{R}$ by

$$\mathcal{E}_H(\varphi) = \sum_{p\in\Lambda^*} \big(|p|^2 |\widehat{\varphi}_p|^2 + \frac{1}{2}\widehat{v}(p) \big| (\widehat{|\varphi|} * \widehat{|\varphi|})_p \big|^2 \big). \tag{3.15}$$

The analogue of Theorem 3.1 reads in the translation invariant setting as follows.

Proposition 3.3. *The Hartree functional $\mathcal{E}_H$ admits, up to multiplication by a constant phase, a unique, normalized minimizer in D_H. The unique positive minimizer $\varphi_H \in D_H$ is given by the constant wave function $\varphi_H = 1_{|\Lambda}$.*

Proof. We may assume without loss of generality that $\widehat{v}(0) > 0$, otherwise there is nothing to prove. Let $\varphi \in D_H$. Since $|\varphi|$ is real-valued, we have $\widehat{|\varphi|}_p \widehat{|\varphi|}_{-p} = \big|\widehat{|\varphi|}_p\big|^2$ s.t.

$$\begin{aligned} \mathcal{E}_H(\varphi) &\geq \inf_{p\in\Lambda^*} (|p|^2 |\widehat{\varphi}_p|^2) + \frac{1}{2}\widehat{v}(0) \big| (\widehat{|\varphi|} * \widehat{|\varphi|})_0 \big|^2 \\ &= \inf_{p\in\Lambda^*} (|p|^2 |\widehat{\varphi}_p|^2) + \frac{1}{2}\widehat{v}(0) \Big(\sum_{q\in\Lambda^*} \widehat{|\varphi|}_q \widehat{|\varphi|}_{-q} \Big)^2 \geq \frac{1}{2}\widehat{v}(0) = \mathcal{E}_H(\varphi_H), \end{aligned}$$

where $\varphi_H = 1_\Lambda$. Hence, φ_H is a normalized minimizer of $\mathcal{E}_H$ in D_H. Moreover, the bound is strict unless $\widehat{\varphi}_p = 0$ for all $p \in \Lambda^* \setminus \{0\}$, that is unless $\varphi = \widehat{\varphi}_0 \varphi_H$ is constant. In that case we have $|\widehat{\varphi}_0| = 1$, by normalization, which proves the claim. □

The last proposition shows that, in the translation invariant setting, the role of the condensate is played by the constant wave function $\varphi_H = 1_{|\Lambda} \in L^2(\Lambda)$. Before we determine the excitation spectrum of H_N, we first introduce a Fock space setting which enables us to focus efficiently on the orthogonal excitations around the condensate.

3.2.1 Fock Space and Excitations around the Condensate

Recall from Example 2.1 that the bosonic Fock space $\mathcal{F} = \mathcal{F}_s\big(L^2(\Lambda)\big)$ is defined by

$$\mathcal{F} = \mathbb{C} \oplus \bigoplus_{k=1}^\infty L_s^2(\Lambda^k).$$

Given a wave function $\psi_N \in L_s^2(\Lambda^N)$ that exhibits complete BEC into some normalized condensate wave function $\varphi_0 \in L^2(\Lambda)$, we know that in the sense of the trace class topology, we have $\psi_N \approx \varphi_0^{\otimes N}$. Instead of considering the part of the wave function ψ_N that describes the condensated particles, we would now like to find a precise description of the fluctuations or excitations around the condensate. Here, we follow the approach introduced in [36] (see, in particular, [36, Section 2.3]) which yields a natural description of the fluctuations of ψ_N around $\varphi_0^{\otimes N}$ as a Fock space vector.

Suppose $\psi_k \in L^2_s(\Lambda^k)$ and $\psi_l \in L^2_s(\Lambda^l)$. Then we define $\psi_k \otimes_s \psi_l \in L^2_s(\Lambda^{k+l})$

$$\begin{aligned}&\psi_k \otimes_s \psi_l(x_1, \ldots, x_{k+l})\\ &\qquad = \frac{1}{\sqrt{k!l!(k+l)!}} \sum_{\sigma \in \mathfrak{S}_{k+l}} \psi_k\big(x_{\sigma(1)}, \ldots, x_{\sigma(k)}\big)\psi_l\big(x_{\sigma(k+1)}, \ldots, x_{\sigma(k+l)}\big)\end{aligned}$$

for *a.e.* $(x_1, \ldots, x_{k+l}) \in \Lambda^{k+l}$. Now, let $\{\varphi_j : j \in \mathbb{N}_0\}$ be a complete orthonormal basis of $L^2_s(\Lambda^N)$ and denote by $L^2_{\perp\varphi_0}(\Lambda) = \operatorname{span}\{\varphi_0\}^\perp$ the orthogonal complement of the space spanned by $\varphi_0 \in L^2(\Lambda)$, as well as by $\mathcal{F}_{\perp\varphi_0} = \mathcal{F}_s(L^2_{\perp\varphi_0}(\Lambda))$. Then, given $\psi_N \in L^2_s(\Lambda^N)$, we can find a unique decomposition

$$\psi_N = \xi^{(0)}\varphi_0^{\otimes N} + \varphi_0^{\otimes N-1} \otimes_s \xi^{(1)} + \varphi_0^{\otimes N-2} \otimes_s \xi^{(2)} + \ldots + \varphi_0^{\otimes} \otimes_s \xi_{N-1} + \xi^{(N)} \tag{3.16}$$

where $\xi^{(k)} \in L^2_{\perp\varphi_0}(\Lambda)^{\otimes_s k}$ for $k = 1, \ldots, N$ and $\xi_0 \in \mathbb{C}$. Indeed, following [32, Section 3.3], let us denote by $p = p(\varphi_0) = |\varphi_0\rangle\langle\varphi_0| \in \mathcal{L}(L^2_s(\Lambda))$ the orthogonal projection onto φ_0 and denote by $q = q(\varphi_0) = 1 - p(\varphi_0) \in \mathcal{L}(L^2_s(\Lambda))$ the projection onto its orthogonal complement. Using these projections, we define the operators $p_k, q_k \in \mathcal{L}(L^2(\Lambda^N))$ by

$$p_k(\varphi_{i_1} \otimes \ldots \otimes \varphi_{i_k} \otimes \ldots \otimes \varphi_{i_N}) = \varphi_{i_1} \otimes \ldots \otimes \big(p_k\varphi_{i_k}\big) \otimes \ldots \otimes \varphi_{i_N}$$

and $q_k = 1 - p_k$, for $k = 1, \ldots, N$. Given any $\psi_N \in L^2_s(\Lambda^N)$, we then have

$$\begin{aligned}\psi_N &= \bigg(\bigotimes_{k=1}^N (p_k + q_k)\bigg)\psi_N = \sum_{\tau \in \{0,1\}^N} \bigotimes_{k=1}^N p_k^{1-\tau_k} q_k^{\tau_k} \psi_N\\ &= \sum_{j=0}^N \sum_{\tau_1 + \cdots + \tau_N = j} \bigotimes_{k=1}^N p_k^{1-\tau_k} q_k^{\tau_k} \psi_N =: \sum_{j=0}^N \psi_N^{(j)}\end{aligned}$$

By the definition of p and q, we certainly have that $\langle \psi_N^{(i)}, \psi_N^{(j)} \rangle = 0$ for all $i \neq j$. Then, defining $\xi^{(j)} \in \big(L^2_{\perp\varphi_0}(\Lambda)\big)^{\otimes_s j}$ by

$$\xi^{(j)}(x_1, \ldots, x_j) = \frac{\sqrt{N!}}{\sqrt{j!(N-j)!}} \big\langle \varphi_0^{\otimes N-j}, \psi_N^{(j)}(x_1, \ldots, x_j, \cdot)\big\rangle_{L^2_s(\Lambda^{N-j})}$$

for *a.e.* $(x_1, \ldots, x_j) \in \Lambda^j$, we conclude that

$$\begin{aligned}\psi_N = \sum_{j=0}^N \psi_N^{(j)} &= \sum_{j=0}^N \frac{1}{j!(N-j)!} \sum_{\sigma \in \mathfrak{S}_N} \sigma\big(q_1 q_2 \ldots q_j p_{j+1} p_{j+2} \ldots p_N \psi_N\big)\\ &= \sum_{j=0}^N \frac{1}{\sqrt{j!(N-j)!N!}} \sum_{\sigma \in \mathfrak{S}_N} \sigma\big(\varphi_0^{\otimes N-j} \otimes \xi^{(j)}\big) = \sum_{j=0}^N \varphi_0^{\otimes N-j} \otimes_s \xi^{(j)}\end{aligned}$$

where $\sigma \in \mathfrak{S}_N$ acts on wave functions in $L^2(\Lambda^N)$ as defined in Section 2.1. This proves (3.16). The representation (3.16) enables us to study the excitation vector

$$(\xi_1, \ldots, \xi_N) \in \mathcal{F}_{\perp\varphi_0}^{\leq N} \hookrightarrow \mathcal{F}_{\perp\varphi_0},$$

describing the fluctations of ψ_N around the pure condensate $\varphi_0^{\otimes N}$. Here, we introduced the notation $\mathcal{F}_{\perp\varphi_0}^{\leq N}$ for the subspace of $\mathcal{F}_{\perp\varphi_0}$ in which each element $\zeta = (\zeta^{(0)}, \zeta^{(1)}, \ldots)$ has components $\zeta^{(k)} = 0$ for all $k > N$. We notice that

$$\begin{aligned}\langle \varphi_0^{\otimes N-j} \otimes_s \xi^{(j)}, \varphi_0^{\otimes N-k} \otimes_s \xi^{(k)} \rangle &= \frac{\delta_{j,k}}{j!(N-j)!N!} \sum_{\sigma,\tau \in \mathfrak{S}_N} \langle \sigma\big(\varphi_0^{\otimes N-j} \otimes \xi^{(j)}\big), \tau\big(\varphi_0^{\otimes N-j} \otimes \xi^{(j)}\big)\rangle \\ &= \frac{\delta_{j,k}}{N!} \sum_{\sigma \in \mathfrak{S}_N} \|\xi^{(j)}\|^2 = \delta_{j,k} \|\xi^{(j)}\|^2.\end{aligned}$$

In particular, (3.16) enables us to define the unitary map $U_N(\varphi_0) : L_s^2(\Lambda^N) \to \mathcal{F}_{\perp\varphi_0}^{\leq N}$

$$U_N(\varphi_0)\psi_N = \big(\xi^{(0)}, \xi^{(1)}, \ldots, \xi^{(N)}\big) \in \mathcal{F}_{\perp\varphi_0}^{\leq N}$$

In view of Proposition 3.3 and the fact that we consider the translation invariant case, we choose for the rest of the section the basis

$$\big\{\varphi_p : p \in 2\pi\mathbb{Z}^3, \varphi_p(x) = e^{ipx} \; \forall x \in \Lambda\big\}$$

so that $\varphi_0 = 1_{|\Lambda}$ plays the role of the condensate wave function. We also abbreviate $U_N = U_N(\varphi_0)$ and $\mathcal{F}_{\perp\varphi_0} = \mathcal{F}_+$, $\mathcal{F}_{\perp\varphi_0}^{\leq N} = \mathcal{F}_+^{\leq N}$ (the + indicates that we consider particles with strictly positive kinetic energy).

When working in the Fock space, where the particle number is not necessarily fixed, it is convenient to introduce the bosonic creation and annihilation operators. For $f, g \in L^2(\Lambda)$, we define the creation operator $a^*(f)$ and the annihilation operator $a(g)$ by

$$\begin{aligned}\big(a^*(f)\zeta\big)^{(n)}(x_1, \ldots, x_n) =& \frac{1}{\sqrt{n}} \sum_{j=1}^{n} f(x_j)\zeta^{(n-1)}(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_n), \\ \big(a(g)\zeta\big)^{(n)}(x_1, \ldots, x_n) =& \sqrt{n+1} \int_\Lambda \overline{g}(x)\zeta^{(n+1)}(x, x_1, \ldots, x_n),\end{aligned}$$

for all $n \in \mathbb{N}$ and

$$\zeta = (\zeta^{(0)}, \zeta^{(1)}, \ldots, \zeta^{(M)}, 0, \ldots) \in \bigcup_{N=0}^{\infty} \mathcal{F}^{\leq N} = \bigcup_{N=0}^{\infty} \bigoplus_{k=0}^{N} L_s^2(\Lambda^k) \subset \mathcal{F}.$$

For $n = 0$, we set $\big(a^*(f)\zeta\big)^{(0)} = 0$.

It is useful to illustrate the action of $a^*(f)$ and $a(f)$ on product states of the basis elements φ_p, $p \in \Lambda^*$. For $\zeta = S_n(\varphi_{p_1} \otimes \varphi_{p_2} \otimes \cdots \otimes \varphi_{p_n}) \in L^2_s(\Lambda^n)$, we have that

$$\begin{aligned} a^*(\varphi_q)\zeta &= \frac{\sqrt{n+1}}{(n+1)!} \sum_{\sigma \in \mathfrak{S}_n} \sum_{j=1}^{n+1} \varphi_{p_{\sigma(1)}} \otimes \cdots \otimes \varphi_{p_{\sigma(j-1)}} \otimes \varphi_q \otimes \varphi_{p_{\sigma(j)}} \otimes \dots \varphi_{p_{\sigma(N)}} \\ &= \sqrt{n+1}\; S_{n+1}(\varphi_q \otimes \varphi_{p_1} \otimes \cdots \otimes \varphi_{p_n}) \in L^2_s(\Lambda^{n+1}) \subset \mathcal{F}^{\leq n+1} \end{aligned}$$

and, similarly, that

$$a(\varphi_q)\zeta = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \langle \varphi_q, \varphi_{p_j} \rangle_2\, S_{n-1}\big(\varphi_{p_1} \otimes \dots \varphi_{p_{j-1}} \otimes \varphi_{p_{j-1}} \otimes \cdots \otimes \varphi_n\big) \in L^2_s(\Lambda^{n-1}) \subset \mathcal{F}^{\leq n-1}.$$

In words, $a^*(\varphi_q)$ creates a particle with momentum $q \in \Lambda^*$ and $a(\varphi_q)$ annihilates a particle with momentum $q \in \Lambda^*$. As a consequence of the last formulae, it follows that

$$a^*(\varphi_q)a(\varphi_q)\zeta = k\zeta,$$

where $0 \leq k \leq n$ denotes the number of the momenta p_j in ζ such that $p_j = q$. Hence, $a^*(\varphi_q)a(\varphi_q) : L^2_s(\Lambda^n) \to L^2_s(\Lambda^n)$ counts the number of particles with momentum $q \in \Lambda^*$. This connects the creation and annihilation operators to the number of excitations.

Basic properties of the creation and annihilation operators are

$$\langle a^*(f)\zeta, \xi \rangle = \langle \zeta, a(f)\xi \rangle$$

for all $\zeta, \xi \in \bigcup_{N=0}^\infty \mathcal{F}^{\leq N}$ so that, at least on a formal level, $a^*(f)$ is the adjoint of $a(f)$. Furthermore, they satisfy the so called canonical commutation relations

$$\big[a(g), a^*(f)\big] = \langle g, f \rangle_2, \qquad \big[a(g), a(f)\big] = 0 \tag{3.17}$$

for all $f, g \in L^2(\Lambda)$. We leave the verification of these properties as an *exercise*.

In the full Fock space $\mathcal{F}$, wave functions can have an arbitrarily large particle number, so it is clear that the creation and annihilation operators are unbounded operators in $\mathcal{F}$. Let us mention that they naturally extend to densely defined, closed and unbounded operators in $\mathcal{F}$. In these notes, however, we restrict our attention to the truncated Fock spaces $\mathcal{F}^{\leq N}$ and, more specifically, on the excitation Fock spaces $\mathcal{F}_+^{\leq N} \hookrightarrow \mathcal{F}^{\leq N}$. Restricted to such truncated spaces, the creation and annihilation operators are bounded and therefore we can ignore the unboundedness issues in the full Fock space $\mathcal{F}$.

Creation and annihilation operators are convenient for computations in the bosonic Fock space, because they implicitly keep track of combinatorial factors due to the symmetry of the wave functions. For computations it is particularly useful to represent basic observables on the Fock space in terms of the creation and annihilation operators. This amounts essentially to nothing more than computing expectation values of observables in a particular basis. Since we work with the standard Fourier basis, let's abbreviate

$$a_p = a(\varphi_p) \qquad \text{and } a^*_q = a^*(\varphi_q)$$

for all $p, q \in \Lambda^* = 2\pi\mathbb{Z}^3$. A particularly important operator in this chapter is the number of particles operator $\mathcal{N}$ which is defined in $\bigcup_{N=0}^{\infty} \mathcal{F}^{\leq N}$ through

$$(\mathcal{N}\zeta)^{(n)} = n\,\zeta^{(n)}, \quad \forall \zeta \in \mathcal{F}^{\leq N}$$

It measures the average number of particles. Observe that $\|\mathcal{N}\|_{\mathcal{L}(\mathcal{F}^{\leq N})} = N$ so, in $\mathcal{F}^{\leq N}$, $\mathcal{N}$ is a bounded operator. Since $\mathcal{N}$ is a multiplication operator, $\mathcal{N}$ is self-adjoint in $\mathcal{F}^{\leq N}$, for every $N \in \mathbb{N}$. By $\mathcal{N}_+$, we denote its restriction to $\bigcup_{N=0}^{\infty} \mathcal{F}_+^{\leq N}$.

Let's express $\mathcal{N}$ in terms of the creation and annihilation operators a_p, a_q^*. From our earlier considerations, we may suspect that in $\bigcup_{N=0}^{\infty} \mathcal{F}^{\leq N}$, we have that

$$\mathcal{N} = \sum_{p \in \Lambda^*} a_p^* a_p.$$

Indeed, to verify this, we can consider w.l.o.g. $\zeta \in L_s^2(\Lambda^n)$ (*why?*) and find that

$$\mathcal{N}\zeta = n\zeta = \sum_{j=1}^n \mathbf{1}_{x_j}\zeta = \sum_{p\in\Lambda^*} \frac{1}{\sqrt{n}} \sum_{j=1}^n \sqrt{n}\big(|\varphi_p\rangle\langle\varphi_p|\big)_{x_j}\zeta = \sum_{p\in\Lambda^*} a_p^* a_p \zeta.$$

and similarly, we find that

$$\mathcal{N}_+ = \sum_{p \in \Lambda_p^* \setminus\{0\}} a_p^* a_p.$$

The following two lemmas are simple, but they are frequently applied in estimating the expectation values of operators in the Fock space.

Lemma 3.1. *Let $f \in L^2(\Lambda)$. Then we have for all $\zeta \in \bigcup_{N=0}^{\infty} \mathcal{F}^{\leq N}$ that*

$$\|a(f)\zeta\| \leq \|f\|_2 \|\mathcal{N}^{1/2}\zeta\|, \quad \|a^*(f)\zeta\| \leq \|f\|_2 \|(\mathcal{N}+1)^{1/2}\zeta\|.$$

Proof. Pick w.l.o.g. $\zeta \in \mathcal{F}^{\leq N}$. We apply Plancherel and Cauchy-Schwarz to obtain that

$$\begin{aligned}
\langle \zeta, a^*(f)a(f)\zeta\rangle &= \sum_{k=0}^N \int_{\Lambda^k} dx_1 \dots dx_k\, \overline{\zeta^{(k)}}(x_1,\dots,x_k) \\
&\qquad \times \sum_{j=1}^k f(x_j) \int_\Lambda dy\, \overline{f}(y)\zeta^{(k)}(y, x_1,\dots,x_{j-1},x_{j+1},\dots,x_k) \\
&\overset{\text{sym.}}{=} \sum_{k=0}^N k \int_{\Lambda^{k-1}} dX \left| \int_\Lambda dy\, \overline{f}(y)\zeta^{(k)}(y,X)\right|^2 \\
&= \sum_{k=0}^N k \int_{\Lambda^{k-1}} dX \left| \sum_{q\in\Lambda^*} \overline{\widehat{f}_p} \int_\Lambda dy\, \overline{\varphi_p}(y)\zeta^{(k)}(y,X)\right|^2 = \sum_{p,q\in\Lambda^*} \widehat{f}_p \overline{\widehat{f}_q} \langle \zeta, a_p^* a_q \zeta\rangle \\
&\leq \sum_{p,q\in\Lambda^*} \big(|\widehat{f}_p|\|a_q\zeta\|\big)\big(|\widehat{f}_q|\|a_p\zeta\|\big) \leq \|f\|_2^2 \sum_{p\in\Lambda^*} \langle\zeta, a_p^* a_p \zeta\rangle = \|f\|_2^2 \langle \zeta, \mathcal{N}\zeta\rangle.
\end{aligned}$$

The second bound follows by noticing that $a(f)a^*(f) = a^*(f)a(f) + \|f\|_2^2$, by (3.17). $\square$

Lemma 3.2. *Let $f \in \ell^2(\Lambda^*)$ and define $A_{(*,*)}(f), A_{(*,\cdot)}(f)$ and $A_{(\cdot,\cdot)}(f)$ by*

$$A_{(*,*)}(f) = \sum_{p\in\Lambda^*} f_p a_p^* a_{-p}^*, \quad A_{(*,\cdot)}(f) = \sum_{p\in\Lambda^*} f_p a_p^* a_p, \quad A_{(\cdot,\cdot)}(f) = \sum_{p\in\Lambda^*} f_p a_p a_{-p}$$

Then, $A_{(*,*)}(f), A_{(*,\cdot)}(f)$ and $A_{(\cdot,\cdot)}(f)$ extend to bounded operators in $\mathcal{F}^{\leq N}$ and we have

$$\|A_{(*,*)}(f)\zeta\|, \ \|A_{(*,\cdot)}(f)\zeta\|, \ \|A_{(\cdot,\cdot)}(f)\zeta\| \ \ \leq \sqrt{2}\|f\|_2\|(\mathcal{N}+1)\zeta\|$$

for all $\zeta \in \mathcal{F}^{\leq N}$. If, in addition $f \in \ell^1(\Lambda^*)$, then also $A_{(\cdot,*)}(f)$, defined by

$$A_{(\cdot,*)}(f) = \sum_{p\in\Lambda^*} f_p a_p a_p^*$$

extends to a bounded operator in $\mathcal{F}^{\leq N}$ with $\|A_{(*,*)}(f)\zeta\| \leq \sqrt{2}\|f\|_2\|(\mathcal{N}+1)\zeta\| + \|f\|_1\|\zeta\|$ for all $\zeta \in \mathcal{F}^{\leq N}$.

Proof. Consider first $A_{(*,*)}(f)$. Then we have

$$\begin{aligned}\|A_{(*,*)}(f)\zeta\|^2 &= \sum_{p,q\in\Lambda^*} \overline{f_p} f_q \langle \zeta, a_p a_{-p} a_q^* a_{-q}^* \zeta\rangle \\ &\leq \sum_{p,q\in\Lambda^*} \overline{f_p} f_q \langle \zeta, (a_q^* a_{-q}^* a_p a_{-p} + 4a_p^* a_q \delta_{p,q} + 4)\zeta\rangle \leq 2\|f\|_2^2 \langle \zeta, (\mathcal{N}+1)^2\zeta\rangle\end{aligned}$$

by Cauchy-Schwarz. The bounds for $A_{(*,\cdot)}(f), A_{(\cdot,\cdot)}(f)$ are analogous. For the non-normally ordered operator $A_{(\cdot,*)}(f)$, we only notice that $a_p a_p^* = a_p^* a_p + 1$, by (3.17). □

The previous two lemmas illustrate that the creation and annihilation operators are quite convenient for operator bounds as long as an upper bound in terms of $\mathcal{N}$ is useful. Below, we also need the kinetic energy $\mathcal{K}_+$ for certain estimates. The operator $\mathcal{K} : \bigcup_{N=0}^\infty \mathbb{C} \oplus \bigoplus_{k=1}^N H_s^2(\Lambda^k) \to \bigcup_{N=0}^\infty \mathcal{F}^{\leq N}$ is the self-adjoint operator defined through

$$(\mathcal{K})_{|\mathcal{N}=n} = \sum_{i=1}^n (-\Delta_{x_i})$$

and with $\mathcal{K}_{|\mathcal{N}=0} = 0$. We denote the restriction of $\mathcal{K}$ to $\bigcup_{N=0}^\infty \mathcal{F}_+^{\leq N}$ by $\mathcal{K}_+$ and we have

$$\mathcal{K}_+ = \sum_{p\in\Lambda^*\setminus\{0\}} |p|^2 a_p^* a_p.$$

The verification of this identity is left as an *exercise*. Similarly, you can check that $\mathcal{K} = \sum_{p\in\Lambda^*} |p|^2 a_p^* a_p$ on a suitable dense domain.

Now, coming back to the Hamiltonian H_N defined in (3.14), we note that $L_s^2(\Lambda^N) \hookrightarrow \mathcal{F}^{\leq N}$. We can also express H_N in terms of the a_p, a_q^* operators, yielding

$$H_N = \bigg(\sum_{p\in\Lambda^*} |p|^2 a_p^* a_p + \frac{1}{2N} \sum_{p,q,r\in\Lambda^*} \widehat{v}(r) a_{p+r}^* a_q^* a_p a_{q+r} \bigg)_{|\mathcal{N}=N}. \tag{3.18}$$

Indeed, for the potential energy, we have by symmetry

$$\begin{aligned}
&\sum_{1\le i<j\le N}\int_{\Lambda^N} dx_1\dots dx_N\, v(x_i-x_j)\overline{\Phi}(x_1,\dots,x_N)\Psi(x_1,\dots,x_N)\\
&=\frac{N(N-1)}{2}\int_{\Lambda^{N-2}}dX\left(\int_{\Lambda^2}dx_1dx_2v(x_1-x_2)\overline{\Phi}(x_1,x_2,X)\Psi(x_1,x_2,X)\right)
\end{aligned}$$

for every $\Phi,\Psi\in L^2_s(\Lambda^N)$ and we can expand this in Fourier space into

$$\begin{aligned}
&\frac{N(N-1)}{2}\int_{\Lambda^{N-2}}dX\int_{\Lambda^2}dx_1dx_2v(x_1-x_2)\overline{\Phi}(x_1,x_2,X)\Psi(x_1,x_2,X)\\
&=N(N-1)\int_{\Lambda^{N-2}}dX\sum_{p,q,s,t\in\Lambda^*}\langle\Phi(\cdot,\cdot,X),\varphi_s\otimes\varphi_t\rangle_{L^2(\Lambda^2)}\langle\varphi_p\otimes\varphi_q,\psi(\cdot,\cdot,X)\rangle_{L^2(\Lambda^2)}\\
&\qquad\times\int_{\Lambda^2}dx_1dx_2v(x_1-x_2)e^{i(p-s)x_1+i(q-t)x_2}\\
&=\sum_{p,q,s,t\in\Lambda^*}\widehat{v}(s-p)\delta_{q,t+s-p}\langle\Phi,a_s^*a_t^*a_pa_q\psi\rangle=\sum_{p,s,t\in\Lambda^*}\widehat{v}(s-p)\langle\Psi,a_s^*a_t^*a_pa_{t+s-p}\psi\rangle\\
&=\sum_{p,q,r\in\Lambda^*}\widehat{v}(r)\langle\Phi,a_{p+r}^*a_q^*a_pa_{q+r}\Psi\rangle,
\end{aligned}$$

where, in the last step, we renamed the variables to $r=s-p$ and $q=t$.

Problem 3.3 (Second quantization of operators)**.** *Let $\boldsymbol{h}$ be a symmetric operator on $L^2(\Omega)$ and let $(\psi_j)_{j\in\mathbb{N}}$ be an orthonormal basis in the domain $D(\boldsymbol{h})$. Show that*

$$\bigoplus_{N=1}^{\infty}\sum_{j=1}^{N}\boldsymbol{h}_{x_j}=\sum_{m,n\in\mathbb{N}}\langle\psi_m,\boldsymbol{h}\psi_n\rangle a^*(\psi_m)a(\psi_n)$$

in the sense of forms on $\bigcup_{N=0}^{\infty}\bigoplus_{k=0}^{N}\bigotimes_{sym}^{k}D(\boldsymbol{h})$. Similarly, assume that V (real-valued) is a multiplication operator in $L^2(\Omega\times\Omega)$ with the property that $V(x,y)=V(y,x)$ for a.e. $(x,y)\in\Omega\times\Omega$. Show that

$$\bigoplus_{N=2}^{\infty}\sum_{1\le i<j\le N}V_{x_i,x_j}=\frac{1}{2}\sum_{m,n,p,q\in\mathbb{N}}\langle\psi_m\otimes\psi_n,V\psi_p\otimes\psi_q\rangle a^*(\psi_m)a^*(\psi_n)a(\psi_p)a(\psi_q).$$

Since we want to focus on the orthogonal excitations of low-energy states, motivated by (3.16), we need to compute the unitarily equivalent excitation Hamiltonian

$$\mathcal{L}_N=U_NH_NU_N^*.$$

This is a simple exercise once we know how U_N acts on the a_p,a_q^* operators.

Problem 3.4. *Check that U_N and its adjoint U_N^* are given by*

$$\begin{aligned} U_N(\psi_N) &= \bigoplus_{k=0}^{N} q^{\otimes k}\bigg(\frac{a_0^{N-k}}{\sqrt{(N-k)!}}\psi_N\bigg), \\ U_N^*\big((\zeta^{(0)},\zeta^{(1)},\dots,\zeta^{(N)})\big) &= \sum_{k=0}^{N}\frac{(a_0^*)^{N-k}}{\sqrt{(N-k)!}}\zeta^{(k)} \end{aligned} \tag{3.19}$$

for all $\psi_N\in L^2_s(\Lambda^N)$ and $\zeta=(\zeta^{(0)},\zeta^{(1)},\dots,\zeta^{(N)})\in\mathcal{F}_+^{\leq N}$. Here, we remind the reader that $q=1-|\varphi_0\rangle\langle\varphi_0|\in\mathcal{L}(L^2(\Lambda))$ (the details can be found in [36, Section 4]).

Given $p,q\in\Lambda_+^*=2\pi\mathbb{Z}^3\setminus\{0\}$, the fact that $[a_p^*a_q,a_0]=[a_p^*a_q,a_0^*]=0$ now implies

$$U_Na_p^*a_qU_N^*=a_p^*a_q,\qquad U_N\mathcal{N}_+U_N^*=\sum_{p\in\Lambda_+^*}a_p^*a_p=\mathcal{N}_+.$$

As a consequence

$$U_Na_0^*a_0U_N^*=U_N(\mathcal{N}-\mathcal{N}_+)U_N^*=U_N(N-\mathcal{N}_+)U_N^*=N-\mathcal{N}_+. \tag{3.20}$$

Finally, for $p\in\Lambda_+^*$, we find with (3.19) for any $\zeta=(\zeta^{(0)},\zeta^{(1)},\dots,\zeta^{(N)})\in\mathcal{F}_+^{\leq N}$ that

$$\begin{aligned} U_Na_p^*a_0U_N^*\zeta &= U_Na_p^*a_0\sum_{k=0}^{N}\frac{(a_0^*)^{N-k}}{\sqrt{(N-k)!}}\zeta^{(k)} = U_N\sum_{k=0}^{N-1}\frac{(a_0^*)^{N-k-1}}{\sqrt{(N-k-1)!}}\sqrt{(N-k)}a_p^*\zeta^{(k)} \\ &= U_N\sum_{k=1}^{N}\frac{(a_0^*)^{N-k}}{\sqrt{(N-k)!}}\big(\sqrt{N-\mathcal{N}_++1}\,a_p^*\,\zeta\big)^{(k)} = U_NU_N^*(a_p^*\sqrt{N-\mathcal{N}_+}\,\zeta). \end{aligned}$$

This means that

$$U_Na_p^*a_0U_N^*=a_p^*\sqrt{N-\mathcal{N}_+},\qquad U_Na_0^*a_qU_N^*=\sqrt{N-\mathcal{N}_+}a_q \tag{3.21}$$

for all $p,q\in\Lambda_+^*$. That is, what the map U_N effectively does is to replace any creation or annihilation operator a_0,a_0^* by $(N-\mathcal{N}_+)^{1/2}$.

We can use the above results to express the property of complete BEC in the Fock space setting. By Lemma 2.14, Eq. (3.20) implies that complete BEC of a sequence $(\psi_N)_{N\in\mathbb{N}}$, $\|\psi_N\|_2=1$, in $L^2_s(\Lambda^N)$ into $\varphi_0\in L^2(\Lambda)$ is equivalent to the condition that

$$\begin{aligned} 1-\langle\varphi_0,\gamma_N^{(1)}\varphi_0\rangle_2 &= 1-\int_{\Lambda^{N-1}}dX\int_{\Lambda^2}dxdy\,\overline{\varphi_0}(x)\psi_N(x,X)\overline{\psi_N}(y,X)\varphi(y) \\ &= 1-\frac{1}{N}\sum_{j=1}^{N}\int_{\Lambda^{N-1}}dX\,\langle\psi_N(\cdot,X),(|\varphi_0\rangle\langle\varphi_0|)_{x_j}\psi_N(\cdot,X)\rangle_{L^2(\Lambda)} \\ &= 1-N^{-1}\langle\psi_N,a_0^*a_0\psi_N\rangle_2=N^{-1}\langle U_N\psi_N,\mathcal{N}_+U_N\psi_N\rangle\to 0 \end{aligned} \tag{3.22}$$

as $N\to\infty$. That is, the expected number of excitations around the condensate is negligible compared to the number of particles in the condensate, in the large N limit.

Finally, having computed the action of U_N on the creation and annihilation operators, a tedious, but straightforward calculation shows that $\mathcal{L}_N = U_N H_N U_N^*$ is given by the sum $\mathcal{L}_N = \mathcal{L}_N^{(0)} + \mathcal{L}_N^{(2)} + \mathcal{L}_N^{(3)} + \mathcal{L}_N^{(4)}$, where

$$
\begin{aligned}
\mathcal{L}_N^{(0)} &= \frac{N}{2}\widehat{v}(0) - \frac{1}{2}\widehat{v}(0) + \frac{\mathcal{N}_+}{2N}\widehat{v}(0) - \frac{\mathcal{N}_+^2}{2N}\widehat{v}(0),\\
\mathcal{L}_N^{(2)} &= \sum_{p\in\Lambda_+^*} \Big[|p|^2 a_p^* a_p + \widehat{v}(p) a_p^* a_p (1-\mathcal{N}_+/N)\Big]\\
&\quad + \frac{1}{2}\sum_{p\in\Lambda_+^*} \widehat{v}(p)\Big[a_p^*(1-\mathcal{N}_+/N)^{1/2} a_{-p}^*(1-\mathcal{N}_+/N)^{1/2} + \text{h.c.}\Big],\\
\mathcal{L}_N^{(3)} &= \frac{1}{N^{1/2}} \sum_{p,q\in\Lambda_+^*: p\neq -q} \widehat{v}(p)\Big[a_{p+q}^*(1-\mathcal{N}_+/N)^{1/2} a_{-p}^* a_q + \text{h.c.}\Big],\\
\mathcal{L}_N^{(4)} &= \frac{1}{2N} \sum_{r\in\Lambda^*,\, p,q\in\Lambda_+^*: p,q\neq -r} \widehat{v}(r) a_{p+r}^* a_q^* a_p a_{q+r}.
\end{aligned}
\tag{3.23}
$$

This follows by splitting the potential energy into a sum of different terms according to their number of zero modes it contains (*why is there no linear term in the* a_p, a_q^**?*).

Problem 3.5. *Verify the identity* (3.23).

In the following, we write $\mathcal{V}_N = \mathcal{L}_N^{(4)}$ for the potential energy of the excited particles, so that $\mathcal{L}_N$ contains in particular the Fock space Hamiltonian $\mathcal{H}_N = \mathcal{K}_+ + \mathcal{V}_N$, measuring the energy of the excitations in different sectors.

3.2.2 Heuristics: Bogoliubov's Method

So far, the introduction of the Fock space setting and the excitation Hamiltonian $\mathcal{L}_N$ is only a translation of the usual $L_s^2(\Lambda^N)$ setting into a different language. Its advantage is that the following heuristics, proposed in a more general setting by N. N. Bogoliubov in [9], becomes particularly transparent.

Suppose we want not only to derive the leading order contribution $\frac{N}{2}\widehat{v}(0)$ to the ground state energy of $\mathcal{L}_N = U_N H_N U_N^*$, but also the next to leading order contribution as well as an approximation of the higher eigenvalues of $\mathcal{L}_N$. How can we proceed? First of all, Bogoliubov assumed that any low-energy wave function ψ_N exhibits complete BEC into the constant wave function $\varphi_0 = 1_{|\Lambda} \in L^2(\Lambda)$. In accordance with (3.22), this implies that the expected number of particles with momentum $p \in \Lambda_+^*$

$$\langle \psi_N, a_p^* a_p \psi_N\rangle = \langle U_N\psi_N, a_p^* a_p U_N \psi_N\rangle \ll N$$

is negligible compared to N, while $\langle \psi_N, a_0^* a_0 \psi_N\rangle \approx N$. As a first approximation, Bogoliubov therefore proposed that the operators a_0, a_0^* in H_N should be replaced by the number $N^{1/2}$. This step is called c-number substitution and it amounts to replace any factor $(N-\mathcal{N}_+)^{1/2}$ in $\mathcal{L}_N$ simply by $N^{1/2}$. The resulting Fock space Hamiltonian consists of a sum of a constant plus several other terms which are either quadratic, cubic or quartic in the creation and annihilation operators of excitations, similar to (3.23). Arguing again via BEC, the cubic and quartic terms should be negligible compared to the remaining contributions, because they are of the order

$$\frac{1}{N^{1/2}}\sum_{p,q\in\Lambda_+^*:p\neq -q}\widehat{v}(p)\Big[a^*_{p+q}a^*_{-p}a_q+\text{h.c.}\Big]\approx O(\mathcal{N}_+^{3/2}/N^{1/2}),$$
$$\frac{1}{2N}\sum_{r\in\Lambda^*,\,p,q\in\Lambda_+^*:p,q\neq -r}\widehat{v}(r)a^*_{p+r}a^*_q a_p a_{q+r}\approx O(\mathcal{N}_+^2/N).$$

If we simply drop these terms, assuming e.g. that $\mathcal{N}_+^2\ll N$, what remains is the operator

$$\mathcal{Q}_N=\frac{N}{2}\widehat{v}(0)-\frac{1}{2}\widehat{v}(0)+\sum_{p\in\Lambda_+^*}\Big[|p|^2a^*_pa_p+\widehat{v}(p)a^*_pa_p+\frac{1}{2}\widehat{v}(p)\big(a^*_pa^*_{-p}+a_pa_{-p}\big)\Big]. \tag{3.24}$$

Notice that $\mathcal{Q}_N$ does not map from $\mathcal{F}_+^{\leq N}$ to itself anymore, but nevertheless we may hope that its spectrum is close to the spectrum of $\mathcal{L}_N$.

Why is the approximation (3.24) useful? The point is that $\mathcal{Q}_N$ can be diagonalized explicitly: the tool which we need is called a Bogoliubov transformation. This is an operator exponential with exponent quadratic in the creation and annihilation operators. Given $(\tau_p)_{p\in\Lambda_+^*}\in\ell^2(\Lambda_+^*)$, we define $T_\tau:\mathcal{F}_+\to\mathcal{F}_+$ by

$$T_\tau=\exp\Bigg[\frac{1}{2}\sum_{p\in\Lambda_+^*}\tau_p\big(a^*_pa^*_{-p}-a_pa_{-p}\big)\Bigg]=\exp(A_\tau). \tag{3.25}$$

Let's compute the action of T_τ on $\mathcal{Q}_N$ without worrying about domain and convergence issues (a more careful analysis follows in the next Section 3.2.3). A simple Taylor expansion together with the canonical commutation relations (3.17) implies

$$\begin{aligned}T^*_\tau a_pT_\tau&=a_p+\int_0^1 ds\;(\partial_s e^{-sA_\tau}a_pe^{sA_\tau})(s)=a_p+\int_0^1 ds\;e^{-sA_\tau}[a_p,A_\tau]e^{sA_\tau}\\&=a_p+\tau_pa^*_{-p}+\int_0^1 ds_1\int_0^{s_2}ds_2\;e^{s_2A_\tau}\big[[a_p,A_\tau],A_\tau\big]e^{-s_2A_\tau}\\&=\cosh(\tau_p)a_p+\sinh(\tau_p)a^*_{-p}.\end{aligned} \tag{3.26}$$

The key of the argument is that a commutator of $a^\sharp_p$ with a quadratic operator is again linear in the creation and annihilation operators, by the commutation relations (3.17).

Choosing $\tau_p=\frac{1}{2}\tanh^{-1}\big(\widehat{v}(p)/[p^2+\widehat{v}(p)]\big)$ and conjugating $\mathcal{Q}_N$ with T_τ, we find

$$\begin{aligned}T^*_\tau\mathcal{Q}_NT_\tau=&\;\frac{N}{2}\widehat{v}(0)-\frac{1}{2}\widehat{v}(0)-\frac{1}{2}\sum_{p\in\Lambda_+^*}\Big[|p|^2+\widehat{v}(p)-\sqrt{|p|^4+2|p|^2\widehat{v}(p)}\Big]\\&+\sum_{p\in\Lambda_+^*}\sqrt{|p|^4+2|p|^2\widehat{v}(p)}\,a^*_pa_p=C_{\mathcal{Q}_N}+\sum_{p\in\Lambda_+^*}\epsilon_pa^*_pa_p.\end{aligned}$$

Hence, the resulting Fock space Hamiltonian is diagonal and we can read off its spectrum. Indeed, we have that

$$U_N^* T_\tau^* \mathcal{Q}_N T_\tau U_N = C_{\mathcal{Q}_N} + \sum_{i=1}^N \mathbf{h}_{x_i},$$

where the one body Hamiltonian $\mathbf{h}$ acts as a Fourier multiplier in $L^2(\Lambda)$, multipliying the p-th Fourier component (for $p \in \Lambda^*$) by

$$\epsilon_p = \sqrt{|p|^4 + 2|p|^2 \widehat{v}(p)}.$$

The ground state energy of $U_N^* T_\tau \mathcal{Q}_N T_\tau^* U_N$ is given by $C_{\mathcal{Q}_N}$ and, by Theorem 2.21, the eigenvalues of $U_N^* T_\tau^* \mathcal{Q}_N T_\tau U_N$ above the ground state energy are given by finite sums

$$\sum_{p \in \Lambda^*} n_p \epsilon_p \; (n_p \in \mathbb{N}_0 \text{ and } n_p \neq 0 \text{ for finitely many } p \in \Lambda^*).$$

Physically, this means that the interacting Bose gas is (up to second order in the energy) equivalent to a non-interacting Bose gas of quasi-particles, via the unitary transformation $T_\tau U_N$. For this reason, one calls the system quasi-free. Instead of the usual one particle kinetic energies $|p|^2, p \in \Lambda_+^*$, the modified excitations have energies

$$\epsilon_p = \sqrt{|p|^4 + 2|p|^2 \widehat{v}(p)}, \; p \in \Lambda_+^*.$$

This incorporates the mean field interaction v through its Fourier transform $\big(\widehat{v}(p)\big)_{p \in \Lambda^*}$.

Let us mention that Bogoliubov's heuristics can be found in many standard physics textbooks on condensed matter (see for instance [41]). From a physical point of view, the important insight from [9] was to provide a microscopic justification of superfluidity which is related to the specific form of the excitation energies ϵ_p.

On the other hand, turning the heuristics into a rigorous proof in specific scaling limits has been an active research field in mathematical physics in recent years, see for instance [63, 30, 36, 5, 6, 12, 50, 15].

3.2.3 Rigorous Derivation of the Excitation Spectrum

The goal of this section is to turn Bogoliubov's heuristics in the mean field regime into a rigorous proof. We follow essentially [63], which provided the first rigorous proof of Bogoliubov's effective theory for mean field bosons, and combine the proof with a few useful arguments from [5, 6].

Let's recall that we assume for simplicity $v \in C_c^\infty\big((-\frac{1}{2}, \frac{1}{2})^3\big)$ to be radially symmetric and such that $\widehat{v}(p) \geq 0$ for all $p \in \Lambda^*$. Our starting point is the excitation Hamiltonian $\mathcal{L}_N$, defined in (3.23). To implement the first step of Bogoliubov's strategy, we need to show that the cubic and quartic contributions, $\mathcal{L}_N^{(3)}$ and $\mathcal{L}_N^{(4)}$, are small on suitable subspaces of low energy vectors. As a first step in this direction, recall that we have the following strong form of complete BEC.

Lemma 3.3. *We have for all $N \in \mathbb{N}$ that*

$$\mathcal{L}_N \geq \frac{N}{2}\widehat{v}(0) + \sum_{p \in \Lambda_+^*} p^2 a_p^* a_p - \frac{1}{2}v(0) = \frac{N}{2}\widehat{v}(0) + \mathcal{K}_+ - \frac{1}{2}v(0) \tag{3.27}$$

Let $(\psi_N)_{N\in\mathbb{N}}$ be a normalized sequence in $D(H_N)$ and define $(\xi_N)_{N\in\mathbb{N}} = (U_N\psi_N)_{N\in\mathbb{N}}$ as the corresponding excitation vectors in $\mathcal{F}_+^{\leq N}$. Assume there exists some $\zeta > 0$ s.t.

$$\langle \xi_N, \mathcal{L}_N \xi_n \rangle \leq \frac{N}{2}\widehat{v}(0) + \zeta$$

Then, by (3.27)*, there exists a constant $C = C(v, \zeta) > 0$, independent of $N \in \mathbb{N}$, s.t.*

$$(4\pi^2)^{-1}\langle \xi_N, \mathcal{N}_+ \xi_N \rangle \ \leq \langle \xi_N, \mathcal{K}_+ \xi_N \rangle \leq C \tag{3.28}$$

In particular, $(\psi_N)_{N\in\mathbb{N}}$ exhibits complete BEC into $\varphi_0 \in L^2(\Lambda)$, by (3.22)*.*

Proof. The bound (3.27) follows by writing out $\sum_{p\in\Lambda_+^*} \widehat{v}(p) \big| \sum_{j=1}^N e^{ipx_j} \big|^2 \geq 0$, implying

$$\frac{1}{N} \sum_{1\leq i<j\leq N} v(x_i - x_j) \geq \frac{N}{2}\widehat{v}(0) - \frac{1}{2}v(0)$$

Conjugating H_N with U_N and using the previous lower bound implies (3.27). □

The previous lemma shows that the kinetic energy of excitation vectors associated to approximate ground state wave functions of H_N is bounded uniformly in N. To get rid of the cubic and quartic terms in $\mathcal{L}_N$, we need, however, stronger a priori bounds.

Proposition 3.4. *Let $(\psi_N)_{N\in\mathbb{N}}$ be a normalized sequence in $D(H_N)$ such that for some $\zeta > 0$ we have $\psi_N = \chi_{(-\infty; \frac{N}{2}\widehat{v}(0)+\zeta]}(H_N)\psi_N$. Also, let $(\xi_N)_{N\in\mathbb{N}} = (U_N\psi_N)_{N\in\mathbb{N}}$. Then, there exists a constant $C > 0$, independent of $N \in \mathbb{N}$, s.t.*

$$\langle \xi_N, \mathcal{N}_+\mathcal{K}_+ \xi_N \rangle \ \leq (C + \zeta)^2 \tag{3.29}$$

Proof. Let's observe first of all that $\mathcal{N}_+$ leaves $D(\mathcal{L}_N)$ invariant. In fact, we have that $D(\mathcal{L}_N) = D(\mathcal{K}_+) = \mathbb{C} \oplus \bigoplus_{k=1}^N H_s^2(\Lambda^k) \cap L_+^2(\Lambda)^{\otimes_s k}$ and the claim follows by noticing that $\mathcal{N}_+$ acts simply as multiplication by k in the k-particle sector of $\mathcal{F}_+^{\leq N}$, $k = 0, \dots, N$. It is clear that $\mathcal{N}_+\mathcal{K}_+$ has the same domain and the operator bound (3.27) implies[11] that

$$\begin{aligned} \mathcal{N}_+\mathcal{K}_+ &= (\mathcal{N}_+ + 1)^{1/2}\mathcal{K}_+(\mathcal{N}_+ + 1)^{1/2} \leq (\mathcal{N}_+ + 1)^{1/2}\widetilde{\mathcal{L}}_N(\mathcal{N}_+ + 1)^{1/2} + C(\mathcal{N}_+ + 1) \\ &= (\mathcal{N}_+ + 1)\widetilde{\mathcal{L}}_N + (\mathcal{N}_+ + 1)^{1/2}[(\mathcal{N}_+ + 1)^{1/2}, \widetilde{\mathcal{L}}_N] + C(\mathcal{N}_+ + 1), \end{aligned} \tag{3.30}$$

where we defined

$$\widetilde{\mathcal{L}}_N = \mathcal{L}_N - \frac{N}{2}\widehat{v}(0).$$

[11] From now on we typically denote generic constants, which may depend on fixed parameters and which may change from line to line, by the symbol C.

Observe that pulling $\widetilde{\mathcal{L}}_N$ to the right in the last step has the advantage that we can control it on low-energy states $\xi_N = \chi_{(-\infty;\zeta]}(\widetilde{\mathcal{L}}_N)$. In fact, for such ξ_N, we use Lemma 3.3 and bound

$$\begin{aligned}\langle \xi_N, (\mathcal{N}_+ + 1)\widetilde{\mathcal{L}}_N \xi_N\rangle &\le \langle \xi_N, (\mathcal{N}_+ + 1)(\widetilde{\mathcal{L}}_N + C)\xi_N\rangle + C\langle \xi_N, (\mathcal{N}_+ + 1)\xi_N\rangle \\ &\le \langle \xi_N, (\mathcal{N}_+ + 1)(\widetilde{\mathcal{L}}_N + C)^{-1}(\mathcal{N}_+ + 1)\xi_N\rangle^{1/2}\langle \xi_N, \widetilde{\mathcal{L}}_N^3 \xi_N\rangle^{1/2} + C \\ &\le \langle \xi_N, (\mathcal{N}_+ + 1)(\widetilde{\mathcal{L}}_N + C)^{-1}(\mathcal{N}_+ + 1)\xi_N\rangle^{1/2}(C+\zeta)^{3/2} + (C+\zeta)\end{aligned}$$

where we chose a sufficiently large $C > 0$ ensuring $\widetilde{\mathcal{L}}_N + C \ge \mathcal{K}_+ + 1 \ge 1$, by (3.27). Next, we use the operator monotonicity of the resolvent[12] to conclude

$$\begin{aligned}\langle \xi_N, (\mathcal{N}_+ + 1)\widetilde{\mathcal{L}}_N \xi_N\rangle &\le \langle \xi_N, (\mathcal{N}_+ + 1)(\mathcal{K}+1)^{-1}(\mathcal{N}_+ + 1)\xi_N\rangle^{1/2}(C+\zeta)^{3/2} + (C+\zeta) \\ &\le \langle \xi_N, (\mathcal{N}_+ + 1)\xi_N\rangle^{1/2}(C+\zeta)^{3/2} + (C+\zeta) \le (C+\zeta)^2\end{aligned} \tag{3.31}$$

This bounds the expectation of the first term on the r.h.s. in (3.30). Let's consider next the commutator term in (3.30). To bound this term, it is convenient to use the identity

$$\frac{1}{\sqrt{s}} = \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}\,\frac{1}{t+s}\,dt$$

for any $s \neq 0$. Using the continuous functional calculus, we write

$$\begin{aligned}[(\mathcal{N}_+ + 1)^{1/2}, \widetilde{\mathcal{L}}_N] &= \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}\,\frac{1}{t+\mathcal{N}_+ + 1}(\mathcal{N}_+ + 1)\widetilde{\mathcal{L}}_N(t+\mathcal{N}_+ + 1)\frac{1}{t+\mathcal{N}_+ + 1}\,dt \\ &\quad - \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}\,\frac{1}{t+\mathcal{N}_+ + 1}(t+\mathcal{N}_+ + 1)\widetilde{\mathcal{L}}_N(\mathcal{N}_+ + 1)\frac{1}{t+\mathcal{N}_+ + 1}\,dt \\ &= \frac{1}{\pi}\int_0^\infty \sqrt{t}\,\frac{1}{t+\mathcal{N}_+ + 1}[\mathcal{N}_+, \widetilde{\mathcal{L}}_N]\frac{1}{t+\mathcal{N}_+ + 1}\,dt\end{aligned}$$

To continue further, we need to have some information on the commutator $[\mathcal{N}_+, \widetilde{\mathcal{L}}_N]$. Going back to (3.23), we notice that $\mathcal{N}_+$ commutes with all, but two contributions to $\widetilde{\mathcal{L}}_N$, namely the non-diagonal quadratic contribution and the cubic contribution. Given $\xi_N = \chi_{(-\infty;\zeta]}(\widetilde{\mathcal{L}}_N)$, these can be estimated with Cauchy-Schwarz by

$$\begin{aligned}&\Big|\sum_{p\in\Lambda_+^*}\widehat{v}(p)\langle \xi_N, [a_p^*(1-\mathcal{N}_+/N)^{1/2}a_{-p}^*(1-\mathcal{N}_+/N)^{1/2} + \text{h.c.}]\xi_N\rangle\Big| \\ &\le 2\|v\|_2\|(\mathcal{N}_+ + 1)^{1/2}\xi_N\|\Big(\sum_{p\in\Lambda_+^*}\langle \xi_N, a_p^* a_{-p}^*(\mathcal{N}_+ + 1)^{-1}a_{-p}a_p\xi_N\rangle\Big)^{1/2} \\ &\le \|v\|_2\langle \xi_N, (\mathcal{N}_+ + 1)\xi_N\rangle\end{aligned}$$

[12]For $0 < A \le B$, we have $\mathbf{1} \le A^{-1/2}BA^{-1/2}$ and hence $A^{1/2}B^{-1}A^{1/2} \le \mathbf{1}$ so that $B^{-1} \le A^{-1}$.

as well as

$$
\begin{aligned}
&\Big|\frac{1}{N^{1/2}}\sum_{p,q\in\Lambda_+^*:p\neq -q}\widehat{v}(p)\langle\xi_N,[a_{p+q}^*(1-\mathcal{N}_+/N)^{1/2}a_{-p}^*a_q+\text{h.c.}]\xi_N\rangle\Big|\\
&\leq\Big(\frac{1}{N}\sum_{p,q\in\Lambda_+^*:p\neq -q}\langle\xi_N,a_{p+q}^*a_{-p}^*a_{-p}a_{p+q}\xi_N\rangle\Big)^{1/2}\Big(\sum_{p,q\in\Lambda_+^*:p\neq -q}\widehat{v}(p)^2\langle\xi_N,a_q^*a_q\xi_N\rangle\Big)^{1/2}\\
&\leq\|v\|_2\langle\xi_N,(\mathcal{N}_++1)\xi_N\rangle.
\end{aligned}
$$

In particular, the previous two bounds imply that

$$-C(\mathcal{N}_++1)\leq i[\mathcal{N}_+,\widetilde{\mathcal{L}}_N]\leq C(\mathcal{N}_++1)$$

for some $C>0$. It follows that the operator

$$\mathcal{A}=(\mathcal{K}_++1)^{-1/2}i[\mathcal{N}_+,\widetilde{\mathcal{L}}_N](\mathcal{K}_++1)^{-1/2}\in\mathcal{L}(\mathcal{F}_+^{\leq N})$$

is bounded in norm by some constant $C>0$, and we conclude that

$$
\begin{aligned}
&|\langle\xi_N,(\mathcal{N}_++1)^{1/2}[(\mathcal{N}_++1)^{1/2},\widetilde{\mathcal{L}}_N]\xi_N\rangle|\\
&\leq\int_0^\infty\sqrt{t}\,\big|\langle(\mathcal{N}_++1)^{1/2}\xi_N,\frac{(\mathcal{K}_++1)^{1/2}}{t+\mathcal{N}_++1}\mathcal{A}\frac{(\mathcal{K}_++1)^{1/2}}{t+\mathcal{N}_++1}\xi_N\rangle\big|\,dt\\
&\leq C\int_0^\infty\frac{\sqrt{t}}{(t+1)^2}\|(\mathcal{K}_++1)^{1/2}(\mathcal{N}_++1)^{1/2}\xi_N\|\|(\mathcal{K}_++1)^{1/2}\xi_N\|\\
&\leq\delta\langle\xi_N,\mathcal{N}_+\mathcal{K}_+\xi_N\rangle+\delta^{-1}C\langle\xi_N,(\mathcal{K}+1)\xi_N\rangle\leq\delta\langle\xi_N,\mathcal{N}_+\mathcal{K}_+\xi_N\rangle+\delta^{-1}(C+\zeta)
\end{aligned}
\tag{3.32}
$$

for any $\delta>0$. Putting (3.30), (3.31) and (3.32) together, we have shown that

$$\langle\xi_N,\mathcal{N}_+\mathcal{K}_+\xi_N\rangle\leq\delta\langle\xi_N,\mathcal{N}_+\mathcal{K}_+\xi_N\rangle+\delta^{-1}(C+\zeta)^2$$

Choosing $0<\delta<1/2$, this proves (3.29). □

What Proposition 3.4 shows is that on spectral subspaces of low enough energy, the expectation of any operator that is dominated by the product of the number of particles $\mathcal{N}_+$ and the kinetic energy $\mathcal{K}_+$ is bounded uniformly in N. Let us now define for all $p\in\Lambda_+^*$ the modified creation and annihilation operators $b_p,b_p^*\in\mathcal{L}(\mathcal{F}_+^{\leq N})$ by

$$b_p=(1-\mathcal{N}_+/N)^{1/2}a_p,\qquad b_p^*=a_p^*(1-\mathcal{N}_+/N)^{1/2}\tag{3.33}$$

We notice that $U_N^*b_pU_N=a_0^*a_p/N^{1/2}$ and $U_N^*b_p^*U_N=a_p^*a_0/N^{1/2}$, so that, on the level of $L_s^2(\Lambda^N)$, the modified creation and annihilation operators either excite a particle from the condensate φ_0 into an excited state φ_p or vice versa. One readily checks that, up to errors of the order $\mathcal{N}_+/N$, which is small on low energy subspaces in view of Proposition 3.4 (and expected to be so in view of Bogoliubov theory), the modified creation and annihilation operators satisfy the canonical commutation relations (3.17). Using these modified fields and estimating the different contributions to $\mathcal{L}_N$ similarly as in the previous proof, we deduce the following corollary.

Corollary 3.1. *$\mathcal{L}_N$, defined in (3.23), is given in form sense on $U_N(\mathcal{D}_N)$ by*

$$\mathcal{L}_N = \frac{N-1}{2}\widehat{v}(0) + \sum_{p\in\Lambda_+^*} \big[p^2 + \widehat{v}(p)\big] b_p^* b_p + \frac{1}{2}\sum_{p\in\Lambda_+^*} \widehat{v}(p)\big[b_p^* b_{-p}^* + b_p b_{-p}\big] + \mathcal{E}_{\mathcal{L}_N} \tag{3.34}$$

where the self-adjoint operator $\mathcal{E}_{\mathcal{L}_N}$ is such that for all $\xi \in D(\mathcal{K}) \cap \mathcal{F}_+^{\leq N}$, we have

$$-CN^{-1/2}\langle \xi, \mathcal{N}_+\mathcal{K}_+\xi\rangle \leq \langle \xi, \mathcal{E}_{\mathcal{L}_N}\xi\rangle \leq CN^{-1/2}\langle \xi, \mathcal{N}_+\mathcal{K}\xi\rangle$$

for some constant $C = C(v) > 0$, which is independent of $N \in \mathbb{N}$. In particular, for low-energy wavefunctions $\xi = \chi_{(-\infty;\zeta]}(\widetilde{\mathcal{L}}_N)\xi \in \mathcal{F}_+^{\leq N}$, we have that

$$-N^{-1/2}(C+\zeta)^2 \leq \langle \xi, \mathcal{E}_{\mathcal{L}_N}\xi\rangle \leq N^{-1/2}(C+\zeta)^2$$

We observe that Corollary 3.1 is a rigorous version of the approximation (3.24), predicted by Bogoliubov theory, with explicit error estimates. The only difference between the quadratic contribution in (3.24) and the quadratic operator in (3.34) is that the usual creation and annihilation operators are replaced by the modified ones, defined in (3.33). The strategy of how to proceed now should be clear from Section 3.2.2. We want to modify the Bogoliubov transformations (3.25) in such a way as to obtain unitary transformations on the excitation Fock space $\mathcal{F}_+^{\leq N}$ with which we can approximately diagonalize the quadratic contribution to $\mathcal{L}_N$, in (3.34).

Comparing with (3.25), the natural guess to approximately diagonalize $\mathcal{L}_N$ is the generalized Bogoliubov transformation

$$e^{B_\tau} = \exp\Big[\frac{1}{2}\sum_{p\in\Lambda_+^*} \tau_p (b_p^* b_{-p}^* - b_p b_{-p})\Big] \tag{3.35}$$

where $(\tau_p)_{p\in\Lambda_+^*} \in \ell^2(\Lambda_+^*)$ is defined by

$$\tau_p = -\frac{1}{2}\tanh^{-1}\big(\widehat{v}(p)/(p^2+\widehat{v}(p))\big) = -\frac{1}{4}\log\Big[1 + 2\frac{\widehat{v}(p)}{p^2}\Big]. \tag{3.36}$$

To verify that (3.35) is indeed a good approach, we proceed as follows. First of all, we need to check that the conjugation of $\mathcal{E}_{\mathcal{L}_N}$ with e^{B_τ} yields an error term, similarly as in Corollary 3.1. Once this is checked, we can proceed to make a rigorous series expansion of $e^{-B_\tau} b_p e^{B_\tau}$, in the spirit of (3.26), keeping track of the error terms. Using the expansions of the conjugated modified creation and annihilation operators, we may expand the quadratic contribution to $\mathcal{L}_N$ to conclude the approximate diagonalization.

Before we start, let us remark that e^{B_τ} leaves $D(\mathcal{L}_N) = D(\mathcal{K}_+)$ invariant. This follows from Lemma 3.2, the identity

$$\sum_{p\in\Lambda_+^*} p^2 a_p^* a_p\, B_\tau = \sum_{p\in\Lambda_+^*} p^2 \tau_p (b_p^* b_{-p}^* + b_p b_{-p}) + B_\tau \sum_{p\in\Lambda_+^*} p^2 a_p^* a_p$$

and the fact that $\sum_{p\in\Lambda_+^*} p^4|\tau_p|^2 \leq \|v\|_2^2 < \infty$.

Lemma 3.4. *For every $l \in \mathbb{N}$, there exists $C > 0$ s.t. for all $\xi \in D(\mathcal{K}_+)$ and $s \in [-1, 1]$*

$$\begin{aligned}
\langle \xi, e^{-sB_\tau}(\mathcal{N}_+ + 1)^l e^{sB_\tau}\xi\rangle &\leq C\langle \xi, (\mathcal{N}_+ + 1)^l \xi\rangle, \\
\langle \xi, e^{-sB_\tau}(\mathcal{N}_+ + 1)(\mathcal{K}_+ + 1)e^{sB_\tau}\xi\rangle &\leq C\langle \xi, (\mathcal{N}_+ + 1)(\mathcal{K}_+ + 1)\xi\rangle, \\
\langle \xi, e^{-sB_\tau}(\mathcal{N}_+ + 1)a_p^* a_p(\mathcal{N}_+ + 1)e^{sB_\tau}\xi\rangle &\leq C\langle \xi, (\mathcal{N}_+ + 1)a_p^* a_p(\mathcal{N}_+ + 1)\xi\rangle \\
&\quad + C|\tau_p|^2\langle \xi, (\mathcal{N}_+ + 1)^3\xi\rangle.
\end{aligned} \tag{3.37}$$

Proof. We prove the second inequality in (3.37), the proof of the other two estimates being similar. For $\xi \in \mathcal{D}(\mathcal{K}_+)$, we consider

$$[0; 1] \ni s \mapsto f_\xi(s) = \langle \xi, e^{-sB_\tau}(\mathcal{N}_+ + 1)(\mathcal{K}_+ + 1)e^{sB_\tau}\xi\rangle$$

and our goal is to apply Gronwall's lemma. We compute

$$(\partial_s f_\xi)(s) = \langle \xi, e^{-sB_\tau}\big[\mathcal{N}_+, B_\tau\big](\mathcal{K}_+ + 1)e^{sB_\tau}\xi\rangle + \langle \xi, e^{-sB_\tau}(\mathcal{N}_+ + 1)\big[\mathcal{K}_+, B_\tau\big]e^{sB_\tau}\xi\rangle$$

Let us bound the second term on the r.h.s. of the last equation. We have

$$\big[\mathcal{K}_+, B_\tau\big] = \sum_{p \in \Lambda_+^*} p^2 \tau_p (b_p^* b_{-p}^* + b_p b_{-p})$$

so that by Cauchy-Schwarz

$$\begin{aligned}
&\big|\langle \xi, e^{-sB_\tau}(\mathcal{N}_+ + 1)\big[\mathcal{K}_+, B_\tau\big]e^{sB_\tau}\xi\rangle\big| \\
&\leq 2\sum_{p \in \Lambda_+^*} |p|\tau_p\| |p| b_{-p}(\mathcal{N}_+ + 2)^{1/2}e^{sB_\tau}\xi\| \|b_p^*(\mathcal{N}_+ + 2)^{1/2}e^{sB_\tau}\xi\| \\
&\leq 2\|v\|_2^2 \|(\mathcal{K}_+ + 1)(\mathcal{N}_+ + 1)e^{sB_\tau}\xi\|^2 \leq C f_{\xi,}(s).
\end{aligned}$$

Arguing analogously for the commutator term containing $\big[\mathcal{N}_+, B_\tau\big]$, we conclude that $(\partial_s f_\xi)(s) \leq C f_\xi(s)$. for some $C > 0$. Notice that the constant $C = C(v)$ is independent of the vector $\xi \in \mathcal{F}_+^{\leq N}$. Gronwall's lemma implies

$$\langle \xi, e^{-sB_\tau}(\mathcal{N}_+ + 1)(\mathcal{K}_+ + 1)e^{sB_\tau}\xi\rangle = f_{\xi,m}(s) \leq e^C f_\xi(0) = e^C\langle \xi, (\mathcal{N}_+ + 1)(\mathcal{K}_+ + 1)\xi\rangle,$$

which proves the second bound in (3.37). □

It follows from the previous lemma that the error operator $\mathcal{E}_{\mathcal{L}_N}$ in (3.34) is still of the order $O(N^{-1})$, in the form sense, after conjugation with e^{B_τ}. The next lemma expands the bounded operator $e^{-B_\tau}b_p e^{B_\tau}$ into a norm-convergent operator series.

Lemma 3.5. *For all $p \in \Lambda_+^*$, there exists a bounded operator $d_p \in \mathcal{L}(\mathcal{F}_+^{\leq N})$ s.t.*

$$e^{-B_\tau}b_p e^{B_\tau} = \cosh(\tau_p)b_p + \sinh(\tau_p)b_{-p}^* + d_p \tag{3.38}$$

and there exists a constant $C > 0$ such that for all $\xi \in \mathcal{F}_+^{\leq N}$, we have that

$$\|d_p\xi\| \leq CN^{-1}\big(\|(\mathcal{N}_+ + 1)a_p\xi\| + \tau_p\|(\mathcal{N}_+ + 1)^{3/2}\xi\|\big). \tag{3.39}$$

Proof. Recall that $B_\tau = \frac{1}{2}\sum_{p\in\Lambda_+^*} \tau_p(b_p^* b_{-p}^* - b_p b_{-p})$ is bounded. We first compute

$$[b_p, B_\tau] = \frac{1}{2}\sum_{q\in\Lambda_+^*} \tau_q [b_p, b_q^* b_{-q}^*] = \tau_p b_{-p}^* - N^{-1}\mathcal{N}_+ \tau_p b_{-p}^* - N^{-1} \sum_{u\in\Lambda_+^*} \tau_u b_{-u}^* a_u^* a_p.$$

By Taylor expanding the function $[0,1] \ni s \mapsto e^{-sB_\tau} b_p e^{sB_\tau}$, this implies

$$e^{-B_\tau} b_p e^{B_\tau} = b_p + \tau_p b_{-p}^* + d_p^{(1)} + \int_0^1 ds_1 \int_0^{s_1} ds_2 \; e^{-s_2 B_\tau} \big[\tau_p b_{-p}^*, B_\tau\big] e^{s_2 B_\tau},$$

where the bounded operator $d_p^{(1)}$ is defined by

$$d_p^{(1)} = -\int_0^1 ds_1 e^{-s_1 B_\tau} \left[N^{-1}\mathcal{N}_+ \tau_p b_{-p}^* + N^{-1} \sum_{u\in\Lambda_+^*} \tau_u b_{-u}^* a_u^* a_p \right] e^{s_1 B_\tau}.$$

Using that $|\tau_p| \le C$ for all $p \in \Lambda_+^*$, and applying Lemma 3.2 and Lemma 3.4, we obtain

$$\|d_p^{(1)}\xi\| \le C N^{-1}\big(\|(\mathcal{N}_+ + 1) a_p \xi\| + \tau_p \|(\mathcal{N}_+ + 1)^{3/2}\xi\|\big)$$

for any $\xi \in \mathcal{F}_+^{\le N}$. Now, we iterate the above procedure. We arrive after $k \in \mathbb{N}$ steps at

$$\begin{aligned} e^{-B_\tau} b_p e^{B_\tau} = & \sum_{j=0}^{\lfloor k/2 \rfloor} \frac{\tau_p^{2j}}{2j!} b_p + \sum_{j=0}^{\lceil (k-1)/2 \rceil} \frac{\tau_p^{2j+1}}{(2j+1)!} b_{-p}^* + \sum_{j=1}^{k} d_p^{(j)} \\ & + \int_0^1 ds_1 \int_0^{s_1} ds_2 \; \dots \int_0^{s_k} ds_{k+1} \; e^{-s_{k+1} B_\tau} [\tau_p^k b_{\flat p}^\sharp, B_\tau] e^{s_{k+1} B_\tau}, \end{aligned}$$

where $(\sharp, \flat) = (*, -)$ if k is odd and $(\sharp, \flat) = (\cdot, +)$ if k is even. Moreover, the operators $d_p^{(j)}$ are given by

$$\begin{aligned} d_p^{(2l)} &= -\,\tau_p^{2l} \int_0^1 ds_1 \dots \int_0^{s_{2l-1}} ds_{2l} \; e^{-s_{2l} B_\tau} \left[\frac{1}{N} b_p \mathcal{N}_+ + \frac{1}{N} \sum_{u\in\Lambda_+^*} \tau_u b_{-u} a_u a_{-p}^* \right] e^{s_{2l} B_\tau}, \\ d_p^{(2l+1)} &= -\,\tau_p^{2l+1} \int_0^1 ds_1 \dots \int_0^{s_{2l}} ds_{2l+1} \; e^{-s_{2l+1} B_\tau} \left[\frac{1}{N} \mathcal{N}_+ b_{-p}^* + \frac{1}{N} \sum_{u\in\Lambda_+^*} \tau_u b_{-u}^* a_u^* a_p \right] e^{s_{2l+1} B_\tau}. \end{aligned}$$

Applying once again Lemma 3.2 and Lemma 3.4, we have for all $\xi \in \mathcal{F}_+^{\le N}$

$$\sum_{j=1}^{k} \|d_p^{(j)}\xi\| \le \sum_{j=1}^{k} \frac{C^k}{k!} N^{-1}\big(\|(\mathcal{N}_+ + 1) a_p \xi\| + \tau_p \|(\mathcal{N}_+ + 1)^{3/2}\xi\|\big)$$

for some fixed $C > 0$, independent of k and N. Similarly, it is simple to see that

$$\int_0^1 ds_1 \int_0^{s_1} ds_2 \; \dots \int_0^{s_k} ds_{k+1} \; e^{-s_{k+1} B_\tau} \|[\tau_p^k b_{\flat p}^\sharp, B_\tau] e^{s_{k+1} B_\tau}\| \le \frac{C^k N^{1/2}}{k!} \to 0 \quad (k \to \infty).$$

Letting $k \to \infty$ and defining $d_p = \sum_{j=1}^\infty d_p^{(j)}$, this proves (3.38) and (3.39). $\square$

We are now ready to approximately diagonalize the Fock space Hamiltonian $\mathcal{L}_N$.

Proposition 3.5. *The excitation Hamiltonian $\mathcal{G}_N = e^{-B_\tau}\mathcal{L}_N e^{B_\tau}$, with $\mathcal{L}_N$ defined in* (3.23) *and B_τ defined in* (3.35), (3.36), *is given in form sense on $U_N(\mathcal{D}_N)$ by*

$$\mathcal{G}_N = \frac{N-1}{2}\widehat{v}(0) - \frac{1}{2}\sum_{p\in\Lambda_+^*}\Big[p^2+\widehat{v}(p)-\sqrt{p^4+2p^2\widehat{v}(p)}\Big] + \sum_{p\in\Lambda_+^*}\sqrt{p^4+2p^2\widehat{v}(p)}\,a_p^*a_p + \mathcal{E}_{\mathcal{G}_N}, \tag{3.40}$$

where the self-adjoint operator $\mathcal{E}_{\mathcal{G}_N}$ is such that for all $\xi \in D(\mathcal{K}_+)\cap\mathcal{F}_+^{\leq N}$, we have

$$-CN^{-1/2}\langle\xi,\mathcal{N}_+\mathcal{K}_+\xi\rangle \leq \langle\xi,\mathcal{E}_{\mathcal{G}_N}\xi\rangle \leq CN^{-1/2}\langle\xi,\mathcal{N}_+\mathcal{K}_+\xi\rangle \tag{3.41}$$

for some constant $C = C(v) > 0$, which is independent of $N\in\mathbb{N}$. In particular, for low-energy wavefunctions $\xi = \chi_{(-\infty;\zeta]}(\mathcal{G}_N - N\widehat{v}(0)/2)\xi \in \mathcal{F}_+^{\leq N}$, we have that

$$-N^{-1/2}(C+\zeta)^2 \leq \langle\xi,\mathcal{E}_{\mathcal{G}_N}\xi\rangle \leq N^{-1/2}(C+\zeta)^2. \tag{3.42}$$

Proof. The proof follows from Corollary 3.1, Lemma 3.4 and Lemma 3.5. Let us indicate the main steps by analyzing first the operator

$$e^{-B_\tau}\Big(\sum_{p\in\Lambda_+^*}p^2b_p^*b_p\Big)e^{B_\tau}.$$

By truncating the sum over $p\in\Lambda_+^*$ first, analyzing the resulting bounded operator via the expansion 3.5 and then removing the truncation using the monotone convergence theorem (recall that $p^2a_p^*a_p \geq 0$ for all $p\in\Lambda_+^*$), we find that

$$\begin{aligned} e^{-B_\tau}\Big(\sum_{p\in\Lambda_+^*}p^2b_p^*b_p\Big)e^{B_\tau} &= \sum_{p\in\Lambda_+^*}p^2\big(\gamma_pb_p^*+\sigma_pb_{-p}+d_p^*\big)\big(\gamma_pb_p+\sigma_pb_{-p}^*+d_p\big)\\ &= \sum_{p\in\Lambda_+^*}p^2\Big[\gamma_p^2b_p^*b_p+\sigma_p^2b_pb_p^*+2\gamma_p\sigma_p(b_p^*b_{-p}^*+b_pb_{-p})\Big]\\ &\quad+\sum_{p\in\Lambda_+^*}p^2\Big[d_p^*\big(\gamma_pb_p+\sigma_pb_{-p}^*\big)+\text{h.c.}\Big]+\sum_{p\in\Lambda_+^*}p^2d_p^*d_p, \end{aligned} \tag{3.43}$$

where we defined $\gamma_p = \cosh(\tau_p)$ and $\sigma_p = \sinh(\tau_p)$. By normal ordering, we find

$$\sum_{p\in\Lambda_+^*}p^2\sigma_p^2b_pb_p^* = \sum_{p\in\Lambda_+^*}p^2\sigma_p^2b_p^*b_p + \sum_{p\in\Lambda_+^*}p^2\sigma_p^2(1-\mathcal{N}_+/N) - N^{-1}\sum_{p\in\Lambda_+^*}p^2\sigma_p^2a_p^*a_p.$$

Using that $\sum_{p\in\Lambda_+^*}p^2\sigma_p^2 \leq C\sum_{p\in\Lambda_+^*}p^2\tau_p^2 \leq C\|v\|_2^2$, it is clear that

$$\Big|N^{-1}\sum_{p\in\Lambda_+^*}p^2\sigma_p^2\langle\xi,\mathcal{N}_+\xi\rangle + N^{-1}\sum_{p\in\Lambda_+^*}p^2\sigma_p^2\langle\xi,a_p^*a_p\xi\rangle\Big| \leq CN^{-1}\langle\xi,(\mathcal{N}_++1)\xi\rangle \tag{3.44}$$

for every $\xi \in D(\mathcal{K}_+)$. Similarly, the two contributions in the last line of (3.43) are error terms. We have for instance for every $\xi \in D(\mathcal{K}_+)$ that

$$\begin{aligned}
&\Big| \sum_{p\in\Lambda_+^*} p^2 \langle \xi, \Big[d_p^* \big(\gamma_p b_p + \sigma_p b_{-p}^*\big) + \text{h.c.}\Big] \xi \rangle \Big| \leq C \sum_{p\in\Lambda_+^*} p^2 \| d_p \xi\| \big(\gamma_p \|b_p \xi\| + \sigma_p \|(\mathcal{N}_+ + 1)^{1/2}\xi\|\big) \\
&\leq CN^{-1} \sum_{p\in\Lambda_+^*} p^2 \big(\|(\mathcal{N}_+ + 1) a_p \xi\| + \tau_p \|(\mathcal{N}_+ + 1)^{3/2}\xi\|\big)\big(\|b_p\xi\| + \tau_p \|(\mathcal{N}_+ + 1)^{1/2}\xi\|\big) \\
&\leq CN^{-1/2} \langle \xi, \mathcal{N}_+ \mathcal{K}_+ \xi\rangle.
\end{aligned}$$

Similarly, we bound the remaining terms in (3.43). Proceeding in the same way for the remaining quadratic contributions to $\mathcal{L}_N$ proves (3.40) after a tedious, but straightforward calculation. The bounds (3.41) and (3.42) are a direct consequence of Lemma 3.4 (applied to $-B_\tau$ instead of B_τ, but it is clear that the proof of Lemma 3.4 does not change when we switch the roles of the operators B_τ by $-B_\tau$). □

The following theorem and its corollary constitute the main results of this section - a rigorous derivation of the excitation spectrum of the mean field Hamiltonian H_N and a norm approximation for the ground state vector of H_N, valid up to errors that vanish in the limit $N \to \infty$ with explicit rates of convergence (cf. [63, 30]).

Theorem 3.3. *Let H_N be as in* (3.14) *and let E_N denote its ground state energy. Then*

$$E_N = \frac{N-1}{2}\widehat{v}(0) - \frac{1}{2}\sum_{p\in\Lambda_+^*} \Big[p^2 + \widehat{v}(p) - \sqrt{p^4 + 2p^2\widehat{v}(p)}\Big] + O(N^{-1/2}) \tag{3.45}$$

Moreover, in the limit of large N, the eigenvalues of $H_N - E_N$ below a given threshold $\zeta > 0$, are given by finite sums of the form

$$\sum_{p\in\Lambda_+^*} n_p \epsilon_p + \mathcal{O}\big(N^{-1/2}(1+\zeta^2)\big), \qquad \epsilon_p = \sqrt{p^4 + 2p^2\widehat{v}(p)} \tag{3.46}$$

where $0 \neq n_p \in \mathbb{N}$ for finitely many $p \in \Lambda_+^*$.

Remark. *Theorem 3.3 can be extended to the inhomogeneous setting, analysing the spectrum of H_N^{trap} as defined in* (3.1) *describing trapped particles, see [30].*

Proof. The proof follows from Proposition 3.5 and the Min-Max Theorem 2.17. Since H_N is unitarily equivalent to $\mathcal{G}_N$, defined in Proposition 3.5, it is enough to compare the min-max values of $\mathcal{G}_N$ with those of the diagonal operator $\mathcal{Q}_N$, defined by

$$\mathcal{Q}_N = \frac{N-1}{2}\widehat{v}(0) - \frac{1}{2}\sum_{p\in\Lambda_+^*} \Big[p^2 + \widehat{v}(p) - \sqrt{p^4 + 2p^2\widehat{v}(p)}\Big] + \sum_{p\in\Lambda_+^*} \sqrt{p^4 + 2p^2\widehat{v}(p)}\, a_p^* a_p.$$

As already indicated in Section 3.2.2, $\mathcal{Q}_N$ is self-adjoint on $\mathcal{D}(\mathcal{K}_+)$ with purely discrete spectrum, given by finite sums of the form

$$\frac{N-1}{2}\widehat{v}(0) - \frac{1}{2}\sum_{p\in\Lambda_+^*} \Big[p^2 + \widehat{v}(p) - \sqrt{p^4 + 2p^2\widehat{v}(p)}\Big] + \sum_{p\in\Lambda_+^*} n_p \epsilon_p.$$

This follows from Theorem 2.21. Note that a complete ONB of eigenvectors of $\mathcal{Q}_N$ is

$$\left\{ \prod_{p\in\Lambda_+^*}^{M} (n_p!)^{-1}(a_p^*)^{n_p}\Omega : n_p \in \mathbb{N}_0 \;\text{ with }\; \sum_{p\in\Lambda_+^*} n_p \le N \right\}$$

and that this set is also a complete set of eigenvectors of $\mathcal{K}_+$. To prove the theorem, we compare the min-max values of $\mathcal{G}_N$ with those of $\mathcal{Q}_N$. To this end, let's denote by $(\lambda_k)_{k\in\mathbb{N}_0}$ the min-max values of $\mathcal{G}_N$ and by $(\mu_k)_{k\in\mathbb{N}_0}$ the min-max values of $\mathcal{Q}_N$, counted with multiplicity. The theorem follows if we can show that

$$|\lambda_k - \mu_k| \le CN^{-1/2}(1+\zeta^2) \tag{3.47}$$

for some $C > 0$, which is independent of N.

Let us start to prove that $\lambda_k \ge \mu_k - CN^{-1/2}(1+\zeta^2)$. First of all, it follows from equations (3.40) and (3.42) that

$$E_N = \lambda_0 = \frac{N-1}{2}\widehat{v}(0) - \frac{1}{2}\sum_{p\in\Lambda_+^*}\left[p^2 + \widehat{v}(p) - \sqrt{p^4 + 2p^2\widehat{v}(p)}\right] + O(N^{-1/2}) = \mu_0 + O(N^{-1/2})$$

Indeed, the upper bound can be obtained by testing $\mathcal{G}_N$ with the vacuum $\Omega \in \mathcal{F}_+^{\le N}$, and the lower bound follows then directly from (3.42). To bound the higher eigenvalues λ_k from below by μ_k, $k \in \mathbb{N}$, we use that $\lambda_k \le \zeta$ and (3.42) to deduce

$$\begin{aligned}\lambda_k &= \inf_{\substack{\dim(V)=k,\\ V=\chi_{(-\infty;\zeta]}(\widetilde{\mathcal{G}}_N)(V)}} \sup_{\xi\in V, \|\xi\|=1} \langle \xi, \mathcal{G}_N \xi\rangle \\ &\ge \inf_{\dim(V)=k} \sup_{\xi\in V,\|\xi\|=1} \langle \xi, \mathcal{Q}_N\xi\rangle - CN^{-1/2}(1+\zeta^2) = \mu_k - CN^{-1/2}(1+\zeta^2),\end{aligned}$$

where we defined $\widetilde{\mathcal{G}}_N = \mathcal{G}_N - E_N$.

On the other hand, to prove that $\lambda_k \le \mu_k + CN^{-1/2}(1+\zeta^2)$, we notice first that the previous bound implies $\mu_k \le \zeta + C$ for N sufficiently large. Then, since we have $\mathcal{N}_+\mathcal{K}_+ \le \mathcal{N}_+(\mathcal{Q}_N - \mu_0) \le (\mathcal{Q}_N - \mu_0)^2$, we easily deduce $\lambda_k \le \mu_k + CN^{-1/2}(1+\zeta^2)$ from (3.40) and (3.41), by testing $\mathcal{G}_N$ on a suitable k-dimensional eigenspace of $\mathcal{Q}_N$ corresponding to its k-th eigenvalue μ_k. □

Corollary 3.2. *Let H_N be as in* (3.14) *and denote by ψ_N a normalized ground state vector*[13] *of H_N, which is unique up to multiplication by a constant phase. Then, there exists some $\omega \in [0, 2\pi)$ and a constant $C > 0$ s.t.*

$$\left\|\psi_N - e^{i\omega}U_N^* e^{B_\tau}\Omega\right\|_2^2 \le C\lambda_1^{-1}N^{-1/2}, \tag{3.48}$$

where λ_1 denotes the first eigenvalue of $H_N - E_N$ above $\lambda_0 = 0$.

[13] Assuming N to be sufficiently large, uniqueness of the ground state vector follows from Theorem 3.3, by noticing that the gap of $H_N - E_N$ is positive.

Proof. We remark that the proof can be extended to eigenvectors with higher eigenvalues, see [30]. We choose $\omega \in [0, 2\pi)$ s.t. $e^{i\omega}\langle \psi_N, U_N^* e^{B_\tau}\Omega\rangle = |\langle \psi_N, U_N^* e^{B_\tau}\Omega\rangle|$. Then (3.48) follows if we can show that

$$1 - |\langle \xi_N, \Omega\rangle|^2 \leq \frac{C}{2\lambda_1} N^{-1/2},$$

where $\xi_N = e^{B_\tau} U_N \psi_N \in \mathcal{F}_+^{\leq N}$. To prove the last bound, we simply observe that

$$\begin{aligned} CN^{-1/2} &\geq \langle \xi_N, (\mathcal{Q}_N - E_N)\xi_N\rangle \geq \langle \xi_N, \big[(\mathcal{Q}_N - E_N)|\Omega\rangle\langle\Omega| + \mu_1(1 - |\Omega\rangle\langle\Omega|)\big]\xi_N\rangle \\ &\geq \lambda_1 \langle \xi_N, (1 - |\Omega\rangle\langle\Omega|)\xi_N\rangle - CN^{-1/2} = \lambda_1(1 - |\langle \xi_N, \Omega\rangle|^2) - CN^{-1/2}. \end{aligned}$$

□

4 Basic Results in the Thermodynamic and GP Limits

The mean field regime considered in the previous section is characterized by very weak interactions. This enables us to obtain strong quantitative statements about BEC and the ground state energy (assuming v to be sufficiently regular). The original paper of Bogoliubov [9], on the other hand, dealt more generally with the usual setting in quantum statistical mechanics of N particles confined to a box $\Lambda_L = [-\frac{L}{2}, \frac{L}{2}]^3$ of side length L. In the thermodynamic limit, one is interested in basic properties of the gas in the limit where the particle density $\rho = N/L^3$ is fixed while the particle number N and the volume $V = L^3$ are both sent to $N, V \to \infty$. This limit is the natural limit in the setting of quantum statistical mechanics, which takes into account temperature and which aims to give precise meaning to the concept of phase transitions.

In these notes, we focus on the ground state energy, which in the language of quantum statistical mechanics corresponds to the setting of zero temperature. For sufficiently small density, one can obtain e.g. the leading order approximation of the ground state energy in the thermodynamic limit. Some aspects of this problem are discussed below. Proving BEC of the ground state in the thermodynamic limit, on the other hand, is a major open problem in mathematical physics. Instead of going into this direction further, we focus on deriving BEC in another scaling regime called the Gross-Pitaevskii (GP) limit. Here, one chooses $L = N$ so that $\rho = \rho_N = 1/N^2 \to 0$ as $N \to \infty$. One can interpret the GP limit as the simplest simultaneous infinite volume and low-density limit, where interactions have a non-trivial effect. In this section, we describe basic results in these two limits: in the thermodynamic limit, we derive an upper bound on the ground state energy (which turns out to be correct to leading order in ρ) and in the Gross-Pitaevskii limit we derive a result on the ground state energy and BEC that is comparable to Theorem 3.2 in the mean field regime.

We start with some heuristics on the ground state energy of the Bose gas and discuss afterwards the proof of the upper bound in the thermodynamic limit. We work in $L^2_s(\Lambda_L^N)$ where $\Lambda_L = [-\frac{L}{2}, \frac{L}{2}]^3$ denotes the box of side length $L > 0$ and the Hamiltonian of the system reads

$$H_N = \sum_{i=1}^{N} (-\Delta)_{x_i} + \sum_{1\le i<j\le N} v(x_i - x_j). \tag{4.1}$$

To focus on the main ideas, we assume for simplicity as before that $v \in C_c^\infty(B_{R_0}) \subset C_c^\infty(\mathbb{R}^3)$ is radial and we also assume that it is pointwise non-negative. Here, $R_0 > 0$ is a fixed parameter (in the thermodynamic limit, notice that $L \sim N^{1/3} \gg R_0$ for N large enough). Our goal is to understand the leading order contribution to the ground state energy E_N at low density ρ. Following our experience with mean field systems, it may seem tempting to conjecture that

$$\psi_N = \varphi_0^{\otimes N} \in L_s^2(\Lambda_L^N), \quad \text{for } \varphi_0 = \frac{1}{L^{3/2}} = \Big(\frac{\rho}{N}\Big)^{1/2} \in L^2(\Lambda_L)$$

yields the right energy to leading order. In other words, we might expect that

$$\lim_{N\to\infty} \frac{E_N}{N} = \langle \psi_N, H_N \psi_N\rangle = \frac{1}{2}\,\rho\,\widehat{v}(0) + o(\rho). \tag{4.2}$$

Here, $\widehat{v}(p) = \int_{\mathbb{R}^3} dx\, e^{-ipx} v(x)$ denotes the Fourier transform of v. This naive mean field prediction (4.2) turns out to be wrong: to obtain the right energy, we need to replace the constant $\widehat{v}(0)$, describing the influence of the potential v to leading order, by another quantity which is called the scattering length $\mathfrak{a}$ of v. This is motivated in the next section. The next theorem follows from [19, 46].

Theorem 4.1. *The ground state energy E_N of H_N, defined in* (4.1)*, satisfies*

$$\lim_{N\to\infty} \frac{E_N}{N} = 4\pi\mathfrak{a}\rho + \mathcal{E},$$

for an error $\mathcal{E} = \mathcal{E}(\rho\mathfrak{a}^3)$ with the property that $\lim_{\rho\mathfrak{a}^3\to 0} \mathcal{E} = 0$.

Remark. *In view of Section 3.2.2, it is worth to note that Bogoliubov's method can be used to predict the second order correction to the ground state energy, which turns out to be of order $O(\rho^{\frac{3}{2}})$. The formula is called Lee-Huang-Yang formula [39, 38] and was recently proved in [68, 28]; see also [2, 29] for related improvements.*

In the following subsections, we introduce the scattering length $\mathfrak{a}$ and the related solution of the zero-energy scattering equation, collect some of its properties, relate it to the two-body problem and prove the upper bound in Theorem 4.1. For the lower bound, see for instance [46, 44, 16, 27]. The last section of this chapter discusses an analogue of Theorem 4.1 and outlines a proof of BEC in the Gross-Pitaevskii limit.

4.1 Heuristics: Scattering Length and Two-Body Problem

Suppose we consider two particles moving in $\mathbb{R}^3$ and interacting through v, the two-body Hamiltonian acting in a suitable dense subspace of $L_s^2(\mathbb{R}^6)$ as

$$H_2 = -\Delta_{x_1} - \Delta_{x_2} + v(x_1 - x_2).$$

To solve the Schrödinger equation, it is suitable to change to relative and center of mass coordinates. The latter coordinates are defined by

$$\mathbf{R} = \frac{1}{2}(x_1 + x_2), \qquad \mathbf{r} = x_1 - x_2.$$

Problem 4.1. *Let $\psi \in C^2(\mathbb{R}^6)$ and let $\Phi : \mathbb{R}^6 \to \mathbb{R}^6$ denote the diffeomorphism defined by $(x_1, x_2) \mapsto \Phi(x_1, x_2) = \big((\boldsymbol{R}(x_1, x_2), \boldsymbol{r}(x_1, x_2)\big)$. Verify that for all $x_1, x_2 \in \mathbb{R}^3$*

$$\big((-\Delta_{x_1} - \Delta_{x_2})(\psi \circ \Phi)\big)(x_1, x_2) = \Big(-\frac{1}{2}\Delta_{\boldsymbol{R}}\,\psi - 2\Delta_{\boldsymbol{r}}\,\psi\Big)(\Phi(x_1, x_2)).$$

In other words, solving the two-body problem with interaction v is the same as solving a one body problem with external potential v (the center of mass dynamics is trivial). So, let's look at the Schrödinger equation for the one body Hamiltonian

$$\mathbf{h} = -\Delta + \frac{1}{2}v,$$

acting on a suitable domain in $L^2(\mathbb{R}^3)$. On a heuristic level, we would like to find a complete set of eigenfunctions of $\mathbf{h}$. Under our assumptions, this can only be understood in a generalized sense[14] like in the free case, where $v = 0$. Indeed, in the latter case the plane waves $x \mapsto \xi_p(x) = e^{2\pi i p x}$, $p \in \mathbb{R}^3$, solve the Schrödinger equation

$$-\Delta\varphi = E\varphi$$

for energies $E = 4\pi^2|p|^2$, and any $\psi \in L^2(\mathbb{R}^3)$ can be expanded in the sense that

$$\psi(x) = \int_{\mathbb{R}^3} dp\,\widehat{\psi}(p)\,e^{2\pi i p x}, \qquad \widehat{\psi}(p) = \int_{\mathbb{R}^3} dx\,e^{-2\pi i p x}\psi(x).$$

Although the $(\xi_p)_{p\in\mathbb{R}^3}$ are not elements in $L^2(\mathbb{R}^3)$ (so that we can not speak of eigenfunctions in the usual sense) they are eigenfunctions in the distributional sense that

$$\int_{\mathbb{R}^3} dx\,e^{-2\pi i p x}(-\Delta\psi)(x) = \widehat{(-\Delta\psi)}(p) = 4\pi^2|p|^2\widehat{\psi}(p) = 4\pi^2|p|^2\int_{\mathbb{R}^3} dx\,e^{-2\pi i p x}\psi(x).$$

Curiously, it turns out that there is an analogous (generalized) eigenfunction expansion for $L^2(\mathbb{R}^3)$ functions in terms of a complete set of eigenfunctions of the one body Hamiltonian $\mathbf{h}$ with potential v. This is a topic in scattering theory, discussed in depth in [57] (including the heuristic discussion of this subsection and its rigorous justification). Physically, the intuition is that for a short range potential v, the state f_p of the interacting system with energy $E = 4\pi^2|p|^2$ should look far in the past like a free state (the so called incoming wave function) of the same energy, that is

$$e^{-it\mathbf{h}}f_p \approx e^{it\Delta}\xi_p$$

[14] The discrete part of the spectrum of $\mathbf{h}$ is empty, see e.g. [31].

for $t \approx -\infty$. Equivalently, $f_p \approx \lim_{t\to-\infty} e^{it\mathbf{h}} e^{it\Delta}\xi_p = \Omega^+\xi_p$. Now, noting that $\Omega^+ = e^{is\mathbf{h}}\,\Omega^+ e^{is\Delta}$ for every $s \in \mathbb{R}$, it follows that $\Omega^+(-\Delta) = \mathbf{h}\,\Omega^+$ and we obtain that

$$\begin{aligned} f_p(x) &\approx e^{-it\Delta} e^{-it(-\Delta+v/2)} f_p(x) + \Big(\frac{i}{2}\int_0^t ds\, e^{-is\Delta}\, v\, e^{-is\mathbf{h}} f_p\Big)(x) \\ &\approx e^{2\pi i p x} + \Big(\frac{i}{2}\lim_{\varepsilon\searrow 0}\int_0^{-\infty} ds\, e^{-is\Delta - is4\pi^2|p|^2 + s\varepsilon}\, v\, f_p\Big)(x) \\ &\approx e^{2\pi i p x} + \frac{1}{2}\Big(\lim_{\varepsilon\searrow 0}\big(-\Delta - 4\pi^2|p|^2 - i\varepsilon\big)^{-1} v\, f_p\Big)(x) \\ &\approx e^{2\pi i p x} - \frac{1}{8\pi}\int_{\mathbb{R}^3} dy\, \frac{e^{2\pi i p(x-y)}}{|x-y|} v(y) f_p(y). \end{aligned}$$

In particular, the state f_p behaves for large $|x| \gg 1$ (to leading order in v) like

$$f_p(x) \approx e^{2\pi i p x} - \frac{e^{2\pi i p x}}{8\pi|x|}\int_{\mathbb{R}^3} dy\, v(y). \tag{4.3}$$

Physically, this is interpreted as saying that a wave function of the interacting system with energy $E = 4\pi^2|p|^2$ consists of the sum of an incoming plane wave and an outgoing spherical wave, the latter describing the scattering effect of the obstacle v (in physics textbooks, (4.3) is commonly the starting point for the discussion of elastic two-body scattering processes, see for instance [37, Chapter XVII]).

How is this discussion useful for the many body problem? Well, at low density, the collision of two particles should be quite rare and it is therefore natural to think of the ground state wave ψ_N of H_N to look like a wave function of the form

$$\psi_N \approx \varphi_0^{\otimes N} \prod_{1\le i<j\le N} f(x_i - x_j).$$

The key question is then what correlation factor f we should use. Motivated by our heuristic discussion above and the fact that we consider the ground state wave function ψ_N of H_N, we would like to use the solution f of the zero energy scattering equation

$$(-2\Delta + v)f = 0 \quad \text{in } \mathbb{R}^3 \quad \text{with} \quad \lim_{x\to\infty} f(x) = 1. \tag{4.4}$$

One can define f rigorously based on the theory of ODE, but here we follow the variational approach as in [44, Appendix C] (valid for a much larger class of potentials v as discussed in these notes, see [44, Appendix C] for the details).

To state the main result on f, we fix some $R > R_0$. Then for $\phi \in H^1(B_R)$, we set

$$\mathcal{E}_R(\phi) = \int_{B_R} dx\, \Big(2|\nabla\phi(x)|^2 + v(x)|\phi(x)|^2\Big). \tag{4.5}$$

Recall that by the trace theorem for Sobolev functions, we can assign $L^2(S_R)$-boundary values to any $\phi \in H^1(B_R)$, where here and in the following $S_R = \partial B_R$.

Proposition 4.1. *The functional (4.5) admits a unique non-negative minimizer in the set $H^1(B_R) \cap \{\phi \in H^1(B_R) : \phi_{|S_R} = 1\}$. Denoting the minimizer by f_R, then f_R is a radially symmetric function, $0 < f_R < 1$ and it satisfies in distributional sense*

$$-2\Delta f_R + v f_R = 0.$$

For $|x| \in (R_0; R]$, f_R is given by

$$f_R(x) = \Big(1 - \frac{\mathfrak{a}}{|x|}\Big) \Big/ \Big(1 - \frac{\mathfrak{a}}{R}\Big) \tag{4.6}$$

for a number $\mathfrak{a}\,(= \mathfrak{a}(v))$, the scattering length of v, which is independent of the choice of $R\,(> R_0)$. Furthermore, we have that

$$\mathcal{E}_R(f_R) = 8\pi\mathfrak{a}/(1 - \mathfrak{a}/R), \qquad \text{and} \qquad \widehat{v}(0) = \int_{\mathbb{R}^3} dx\, v(x) > 8\pi\mathfrak{a} \ \ (\text{if } v \neq 0). \tag{4.7}$$

Proof. We use the direct methods of the calculus of variations. We start with a minimizing sequence $(\phi_j)_{j\in\mathbb{N}}$ in $H^1(B_R)\cap\{\phi \in H^1(B_R) : \phi_{|S_R} = 1\}$. By Prop. 3.1, we can assume that the ϕ_j are non-negative (if not, we can replace each ϕ_j by $|\phi_j|$ which only lowers the energy). Furthermore, by replacing ϕ_j if necessary by $\min(\phi_j, 1_{|B_R}) \in H^1(B_R)$, we can assume that $\phi_j \leq 1$ for all $j \in \mathbb{N}$, and noticing that $1_{|B_R} - \phi_j \in H^1_0(B_R)$, we can also assume w.l.o.g. that $1_{|B_R} - \phi_j \in C_c^\infty(B_R)$, by density of $C_c^\infty(B_R) \subset H^1(B_R)$. Finally, using once again the convexity of the map $\rho \mapsto \|\nabla\sqrt{\rho}\|_2^2$, we can assume that each ϕ_j is radially symmetric, replacing it by the spherical average

$$B_R \ni x \mapsto \sqrt{\frac{1}{|S_{|x|}|}\int_{S_{|x|}} d\omega\, |\phi_j|^2}$$

if necessary. Next, we notice that the sequence (ϕ_j) is bounded in $H^1(B_R)$ and has a weakly convergent subsequence, denote its limit by $f_R \in H^1(B_R)$. By the compact embedding $H^1(B_R) \hookrightarrow L^2(B_R)$, we can also assume that ϕ_j converges to f_R pointwise almost surely so that in particular $0 \leq f_R \leq 1$. Furthermore, since $1_{|B_R} - \phi_j \in C_c^\infty(B_R)$ for all $j \in \mathbb{N}$, we must have that $1_{|B_R} - f_R \in H^1_0(B_R)$, that is, $(f_R)_{|S_R} = 1$. Now, the functional $\mathcal{E}_R$ is weakly sequentially lower semi-continuous (*exercise*), so that

$$\mathcal{E}_R(f_R) = \inf_{\phi\in H^1(B_R)\cap\{\phi\in H^1(B_R):\phi_{|S_R}=1\}} \mathcal{E}_R(\phi).$$

That is, f_R is a minimizer of $\mathcal{E}_R$. The Euler-Lagrange equation follows as usual by differentiating $t \mapsto \mathcal{E}_R(f_R + t\xi)$ at $t = 0$, for a given $\xi \in C_c^\infty(B_R)$. This implies that

$$-2\Delta f_R + v f_R = 0.$$

By elliptic regularity, f_R is continuous and since $v f_R \geq 0$, f_R is subharmonic (for the definition and basic properties, we refer to [40, Chapter 9]). Subharmonic functions satisfy the maximum principle (see [40, Theorem 9.3]) which tells us that either $f_R < 1$

in B_R or $f_R = 1$ in B_R. Since we exclude the trivial case that $v = 0$, we must have $f_R < 1$ in B_R. That $f_R > 0$ follows as in the proof of Prop. 3.2 and then, the uniqueness of f_R follows from the convexity inequality for gradients, Prop. 3.1.

The specific form (4.6) of f_R can be seen as follows. In the annulus $|x| \in (R_0; R]$, f_R is a harmonic function, i.e. $\Delta f_R = 0$ (in particular, f_R is smooth in this annulus). The only smooth, radial solutions in $\mathbb{R}^3$ to this equation are of the form $x \mapsto c_1 + c_2|x|^{-1}$ (*why?*), where one of the constants is fixed by the boundary condition on S_R. This means f_R can be written as in (4.6) for some $\mathfrak{a}$, which may a priori depend on R.

Let's check that $\mathfrak{a}$ is independent of R. If not, we would find $R < \widetilde{R}$ and solutions $f_R, f_{\widetilde{R}}$ both having the form (4.6) in the regions where $|x| \in (R_0; R]$ and $|x| \in (R_0; \widetilde{R}]$, respectively. Defining a new function $g_{\widetilde{R}} \in H^1(B_{\widetilde{R}})$ via

$$g_{\widetilde{R}}(x) = \begin{cases} f_{\widetilde{R}}(R) f_R(x) & \text{if } |x| \leq R, \\ f_{\widetilde{R}}(x) & \text{if } R < |x| \leq \widetilde{R}, \end{cases}$$

we can only have that $\mathcal{E}_{\widetilde{R}}(g_{\widetilde{R}}) \leq \mathcal{E}_{\widetilde{R}}(f_{\widetilde{R}})$ (*why?*), so by the uniquness, we conclude that $g_{\widetilde{R}} = f_{\widetilde{R}}$ which also implies that $\mathfrak{a}(R) = \mathfrak{a}(\widetilde{R}) = \mathfrak{a}$.

An important observation implied by the previous argument is that the function

$$x \mapsto (1 - \mathfrak{a}/R) f_R(x)$$

is independent of $R > R_0$. In particular, we can define the solution $f : \mathbb{R}^3 \to \mathbb{R}$ of the zero-energy scattering equation (4.4) as the limit

$$f(x) = \lim_{R\to\infty} (1 - \mathfrak{a}/R) f_R(x).$$

Then f clearly solves (4.4) and it equals

$$f(x) = 1 - \frac{\mathfrak{a}}{|x|},$$

for $|x| > R_0$ so that $\lim_{x\to\infty} f(x) = 1$, as desired.

Finally, let us explain (4.7). The energy formula follows from

$$\mathcal{E}_R(f_R) = 2\int_{S_R} d\omega\, \nabla f_R \cdot \frac{x}{|x|} + \int_{B_R} dx\, f_R(x)\Big(-2\Delta f_R(x) + \frac{1}{2} v(x) f_R(x)\Big) = \frac{8\pi\mathfrak{a}}{1 - \mathfrak{a}/R},$$

while the bound on $\widehat{v}(0)$ follows from $\widehat{v}(0) = \mathcal{E}_R(1_{|B_R}) \geq \mathcal{E}_R(f_R) > 8\pi\mathfrak{a}$. □

Problem 4.2. *Let f denote the solution of* (4.4)*. Prove that*

$$8\pi\mathfrak{a} = \int_{\mathbb{R}^3} dx\, v(x) f(x).$$

Problem 4.3. *Show that the solution f of* (4.4) *is increasing in $|x|$. Moreover, show that for all $x \in \mathbb{R}^3$, we have that*

$$f(x) \geq \max\Big[1 - \frac{\mathfrak{a}}{|x|}, 0\Big].$$

Hint: Use the maximum principle for subharmonic functions.

Problem 4.4. *Let $v = \lambda \chi_{B_{R_0}(0)}$ be a box potential of strength $\lambda > 0$ and range $R_0 > 0$. Compute its scattering length $\mathfrak{a}$ explicitly in terms of λ and R_0.*

The scattering length has the following interpretation. It follows from Proposition 4.1 that $\mathfrak{a} < R$, the range of v. On the other hand, if one considers a hard core potential

$$v_{\mathrm{hc}} = \begin{cases} \infty & \text{if } |x| \le R, \\ 0 & \text{else}, \end{cases}$$

one can check that the solution of the scattering equation (4.4) is given by

$$f_{\mathrm{hc}} = \begin{cases} 0 & \text{if } |x| \le R, \\ 1 - \mathfrak{a}^{\mathrm{hc}} |x|^{-1} & \text{else}. \end{cases}$$

In particular, by continuity, we see that $\mathfrak{a}^{\mathrm{hc}} = R$. The interpretation is that if two particles interact via v and we want to ignore the details of v, but replace it for simplicity with a hard-core box potential, the best range to choose is the scattering length $\mathfrak{a}(v)$.

We close this section with a basic result that explains why (4.2) cannot expected to be correct. To this end, consider two bosons moving in $\Lambda_L = \mathbb{R}^3/L\mathbb{Z}^3$ and interacting through $v \in C_c^\infty(B_R(0))$, $v \ge 0$ for some small $R > 0$. Thus, the state of the system is described by a wave function in $L^2_s(\Lambda_L^2)$. Denote by $E_{2,L}$ the ground state energy of

$$H_{2,L} = -\Delta_{x_1} - \Delta_{x_2} + v(x_1 - x_2).$$

Then, we have the following asymptotics for $E_{2,L} = \inf \sigma(H_{2,L})$, as $L \to \infty$.

Lemma 4.1. *There exists an error $o(1)$ that satisfies $\lim_{L\to\infty} o(1) = 0$ so that*

$$E_{2,L} = 8\pi \mathfrak{a} L^{-3}\big(1 \ + o(1)\big). \tag{4.8}$$

Proof. To use the same notation as in Section 3.2, note that (4.8) is equivalent to

$$e_{2,L} = \inf \sigma\big(- \Delta_{x_1} - \Delta_{x_2} + L^2 v(L(x_1 - x_2))\big) = 8\pi \mathfrak{a} L^{-1}\big(1 \ + o(1)\big) \tag{4.9}$$

for a system of two bosons moving in $\mathbb{T}^3$ and interacting through the rescaled potential $L^2 v(L.)$, by a simple change of variables. Let's abbreviate in the sequel

$$\mathbf{h} = -\Delta_{x_1} - \Delta_{x_2} + v_L,$$

where v_L denotes the multiplication operator $L^2 v(L(x_1 - x_2))$ in $L^2_s(\mathbb{T}^3 \times \mathbb{T}^3)$.

The proof of (4.9) is based on some recent ideas introduced in [17, Section 2]; see also [11]. It uses the Schur complement formula and it consists of three main steps:

(1) Prove BEC of the ground state ψ_{gs} through a simple energy upper bound.

(2) Use the a priori information on BEC to prove the correct energy lower bound.

(3) Construct a related trial state to derive the correct energy upper bound.

To prove an a priori bound on the number of orthogonal excitations, notice that

$$\langle\psi_{\rm gs},\mathcal{N}_+\psi_{\rm gs}\rangle \leq \langle\psi_{\rm gs},(-\Delta_{x_1}-\Delta_{x_2})\psi_{\rm gs}\rangle \leq e_{2,L} \leq \langle\varphi_0\otimes\varphi_0,\mathbf{h}\,\varphi_0\otimes\varphi_0\rangle = \frac{\widehat{v}(0)}{L}. \tag{4.10}$$

The bound (4.10) implies that for the ground state $\psi_{\rm gs}$, the number of particles in the condensate state $\varphi_0 = 1_{|\mathbb{T}^3} \in L^2(\mathbb{T}^3)$ is bounded from below by

$$\langle\psi_{\rm gs}, a_0^*a_0\psi_{\rm gs}\rangle = 2 - \langle\psi_{\rm gs},\mathcal{N}_+\psi_{\rm gs}\rangle \geq 2 - L^{-1}\,\widehat{v}(0).$$

Now, define the projections $\Pi_0 = |\varphi_0\otimes\varphi_0\rangle\langle\varphi_0\otimes\varphi_0|$ and $\Pi_+ = 1-\Pi_0$. By the Schur complement formula from linear algebra, it is straightforward to verify the identity

$$\begin{aligned}&\mathbf{h} = (1+\mathbf{s}^*)\big(-\Delta_{x_1}-\Delta_{x_2}+\Pi_0 v_{\rm ren}\Pi_0 + \Pi_+ v_L\Pi_+\big)(1+\mathbf{s}), \quad \text{where}\\ &\mathbf{s} = \Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+ v_L\Pi_0, \ \ v_{\rm ren} = v_L - v_L\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+ v_L.\end{aligned} \tag{4.11}$$

Notice here that $\Pi_+\mathbf{h}\,\Pi_+ \geq 4\pi^2\Pi_+$ (using that $v\geq 0$ pointwise) so that $\Pi_+\mathbf{h}\,\Pi_+$ is invertible as a map from $\Pi_+L^2_s(\mathbb{T}^3\times\mathbb{T}^3)$ to itself. Note, moreover, that $\Pi_0\,\mathbf{s} = \mathbf{s}^2 = 0$.

On a heuristic level, we may expect that $\mathbf{h}\,\mathbf{s}\approx v_L$, which should be compared to the zero energy scattering equation, which is equivalent to $(-2\Delta+v_L)(1-f_L) = v_L$. In other words, we may expect that $\mathbf{s}$, a translation invariant operator on $L^2_s(\mathbb{T}^3\times\mathbb{T}^3)$, is close to the multiplication operator s_L that multiplies by $(1-f(L(x_1-x_2))$ in $L^2_s(\mathbb{T}^3\times\mathbb{T}^3)$. Below, we use this observation. Before doing so, note first that (4.11) implies

$$\mathbf{h} \geq \Pi_0 v_{\rm ren}\Pi_0 = \frac{1}{2}\langle\varphi_0\otimes\varphi_0, v_{\rm ren}\varphi_0\otimes\varphi_0\rangle a_0^*a_0^*a_0a_0.$$

Using (4.10) and the identity $a_0^*a_0 = 2-\mathcal{N}_+$, we obtain

$$\begin{aligned}\langle\psi_{\rm gs},\mathbf{h}\psi_{\rm gs}\rangle &\geq \frac{1}{2}\langle\varphi_0\otimes\varphi_0, v_{\rm ren}\varphi_0\otimes\varphi_0\rangle\langle\psi_{\rm gs},(2-\mathcal{N}_+)(1-\mathcal{N}_+)\psi_{\rm gs}\rangle\\ &\geq \langle\varphi_0\otimes\varphi_0, v_{\rm ren}\varphi_0\otimes\varphi_0\rangle(1-CL^{-1}).\end{aligned} \tag{4.12}$$

Based on the above heuristic remark on $\mathbf{s}$, we now expect that

$$\langle\varphi_0\otimes\varphi_0, v_{\rm ren}\varphi_0\otimes\varphi_0\rangle = \langle\varphi_0\otimes\varphi_0, v_L(1-\mathbf{s})\varphi_0\otimes\varphi_0\rangle \approx \int dx\, L^2(vf)(Lx) = 8\pi\mathfrak{a}L^{-1},$$

and our next task is to make this rigorous. To this end, let f denote the solution of (4.4), let $\chi\in C_c^\infty(B_{\frac{1}{2}}(0))$ be a non-negative, radial bump function s.t. $\chi_{|B_{\frac{1}{4}}(0)} = 1$ and

$$f_L(x_1,x_2) = \chi(x_1-x_2)f(L(x_1-x_2)),\ s_L(x_1,x_2) = (1-f_L)(x_1,x_2).$$

In particular, both $f_L, s_L\in L^2_s(\mathbb{T}^3\times\mathbb{T}^3)$ are in the domain of $\mathbf{h}$ (which is the same as the domain of $-\Delta_{x_1}-\Delta_{x_2}$). Viewing s_L as a multiplication operator, we have that

$$\begin{aligned}\mathbf{h}\,s_L &= v_L - 4L^{-1}\mathfrak{a}\frac{x_1-x_2}{|x_1-x_2|^3}\cdot(\nabla\chi)(x_1-x_2) - 2L^{-1}\mathfrak{a}\frac{(\Delta\chi)(x_1-x_2)}{|x_1-x_2|}\\ &= v_L + L^{-1}\widetilde{\chi}(x_1-x_2).\end{aligned}$$

for L large enough. Notice that $\widetilde{\chi} \in C_c^\infty\big(B_{\frac{1}{2}}(0) \setminus B_{\frac{1}{4}}(0)\big)$. Identifying $\widetilde{\chi}$ with the multiplication operator $\widetilde{\chi}(x_1 - x_2)$ in $L^2_s(\mathbb{T}^3 \times \mathbb{T}^3)$, the last identity implies that

$$\begin{aligned}
\mathbf{s}\,\varphi_0 \otimes \varphi_0 &= \Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+ v_L\varphi_0 \otimes \varphi_0 \\
&= \Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+\mathbf{h}\, s_L\varphi_0 \otimes \varphi_0 - L^{-1}\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+\widetilde{\chi}\varphi_0 \otimes \varphi_0 \\
&= s_L\varphi_0 \otimes \varphi_0 - \Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+\mathbf{h}\Pi_0\, s_L\varphi_0 \otimes \varphi_0 \\
&\quad - \Pi_0 s_L\varphi_0 \otimes \varphi_0 - L^{-1}\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+\widetilde{\chi}\varphi_0 \otimes \varphi_0
\end{aligned}$$

and thus

$$\begin{aligned}
&\langle \varphi_0 \otimes \varphi_0, v_{\mathrm{ren}}\varphi_0 \otimes \varphi_0\rangle \\
&= 8\pi\mathfrak{a}L^{-1} + \langle \varphi_0 \otimes \varphi_0, v_L\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+\mathbf{h}\,\varphi_0 \otimes \varphi_0\rangle\langle \varphi_0 \otimes \varphi_0, s_L\varphi_0 \otimes \varphi_0\rangle \\
&\quad + L^{-1}\widehat{v}(0)\langle \varphi_0 \otimes \varphi_0, s_L\varphi_0 \otimes \varphi_0\rangle + L^{-1}\langle \varphi_0 \otimes \varphi_0, v_L\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+\widetilde{\chi}\varphi_0 \otimes \varphi_0\rangle.
\end{aligned}$$

Based on Problem 4.5, we conclude that

$$0 \le L^{-1}\widehat{v}(0)\langle \varphi_0 \otimes \varphi_0, s_L\varphi_0 \otimes \varphi_0\rangle \le CL^{-2}\int_{\mathbb{T}^3\times\mathbb{T}^3}\frac{dx_1dx_2}{|x_1 - x_2|} \le CL^{-2}.$$

Using this bound and Cauchy-Schwarz, we obtain that

$$\begin{aligned}
0 &\le \langle \varphi_0 \otimes \varphi_0, v_L\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+\mathbf{h}\,\varphi_0 \otimes \varphi_0\rangle\langle \varphi_0 \otimes \varphi_0, s_L\varphi_0 \otimes \varphi_0\rangle \\
&\le CL^{-1}\Big\langle v_L^{\frac{1}{2}}\varphi_0 \otimes \varphi_0, \Pi_+ v_L^{\frac{1}{2}}\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+ v_L^{\frac{1}{2}}\Pi_+\, v_L^{\frac{1}{2}}\varphi_0 \otimes \varphi_0\Big\rangle \\
&\qquad + CL^{-1}\Big\langle v_L^{\frac{1}{2}}\varphi_0 \otimes \varphi_0, \Pi_0 v_L^{\frac{1}{2}}\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+ v_L^{\frac{1}{2}}\Pi_0 v_L^{\frac{1}{2}}\varphi_0 \otimes \varphi_0\Big\rangle \\
&\le CL^{-2}\widehat{v}(0) + CL^{-1}\Big\langle v_L^{\frac{1}{2}}\varphi_0 \otimes \varphi_0, \Pi_0 v_L\Pi_0 v_L^{\frac{1}{2}}\varphi_0 \otimes \varphi_0\Big\rangle \le CL^{-2}.
\end{aligned}$$

Finally, we use that $v_L\varphi_0 \otimes \varphi_0 = \mathbf{h}\,\varphi_0 \otimes \varphi_0$ so that

$$L^{-1}\big|\ \langle \varphi_0 \otimes \varphi_0, v_L\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-1}\Pi_+\widetilde{\chi}\varphi_0 \otimes \varphi_0\rangle\big| \le CL^{-1}\|\mathbf{s}\|_{\mathrm{op}}$$

and arguing similarly as in the previous step, we find

$$\|\mathbf{s}\|^2_{\mathrm{op}} = \langle \varphi_0 \otimes \varphi_0, v_L\Pi_+\big(\Pi_+\mathbf{h}\,\Pi_+\big)^{-2}\Pi_+ v_L\varphi_0 \otimes \varphi_0\rangle \le CL^{-1}.$$

Collecting the above estimates and inserting them into (4.12) shows that

$$e_{2,L} \ge 8\pi\mathfrak{a}L^{-1}\big(1\ - CL^{-\frac{1}{2}}\big).$$

This proves the correct energy lower bound. To finish the proof, it remains to prove the corresponding ground state energy upper bound. To this end, we need to find a suitable trial state. Motivated by the above computations, it should be obvious that

$$\psi = \frac{(1 - \mathbf{s})\varphi_0 \otimes \varphi_0}{\|(1 - \mathbf{s})\varphi_0 \otimes \varphi_0\|}$$

is a good candidate. Indeed, $\|(1-\mathbf{s})\varphi_0 \otimes \varphi_0\| \geq 1 - CL^{-\frac{1}{2}}$ and using that

$$\mathbf{h}\,(1-\mathbf{s})\varphi_0 \otimes \varphi_0 = \langle \varphi_0 \otimes \varphi_0, v_{\mathrm{ren}}\varphi_0 \otimes \varphi_0 \rangle (1+\mathbf{s}^*)\varphi_0 \otimes \varphi_0,$$

it is straightforward to show that $e_{2,L} \leq \langle \psi, \mathbf{h}\,\psi \rangle \leq 8\pi\mathfrak{a}L^{-1}\big(1+CL^{-1}\big)$. This proves the ground state energy formula (4.9) for an error which is bounded by $|o(1)| \leq CL^{-\frac{1}{2}}$. $\square$

Problem 4.5. *Let f denote the solution of the zero energy scattering equation* (4.4) *for v as above. Show that $w = 1-f$ satisfies for some $C > 0$ the bounds*

$$|w(x)| \leq \frac{C}{1+|x|}, \quad |\widehat{w}(p)| \leq \frac{C}{1+|p|^2}.$$

What Lemma 4.1 demonstrates is that the naive conjecture (4.2) is not even correct for a system of two particles that interact in a large volume through a regular short range potential v. Two body correlations that are caused by the interaction lower the ground state energy in a non-trivial way and we should not expect that this picture becomes simpler in case of N interacting particles. Indeed, a more reasonable conjecture than (4.2) is that the ground state energy E_N of the N-body system equals to leading order in the density $\rho = NL^{-3}$ the two-body ground state energy times the number of pairs of particles that can be formed from N particles. This provides a possible interpretation for the formula in Theorem 4.1, which turns out to be correct for dilute systems.

4.2 Ground State Energy Upper Bound in Thermodynamic Limit

Following the heuristic discussion from the last section, we now switch to the proof of the upper bound for Theorem 4.1, following [44, Theorem 2.2]. We denote by $\mathfrak{a}$ the scattering length of v and consider H_N in (4.1) with periodic boundary conditions.

Theorem 4.2. *If the diluteness parameter $Y = \rho\mathfrak{a}^3$ is small enough, we have that*

$$\frac{E_N}{N} \leq 4\pi\mathfrak{a}\rho\big(1 + O(Y^{\frac{1}{3}})\big).$$

Remark. *The parameter $\rho^{\frac{1}{3}}\mathfrak{a}$ is a diluteness parameter for the gas: $\rho^{-\frac{1}{3}}$ corresponds to the average distance between two particles and $\mathfrak{a}$ to the effective range of v.*

Proof. The theorem follows by constructing a suitable trial state. We will construct a vector which is not symmetric under permutations of the particles. The reason why this is no problem is that the positive ground state ψ_N of H_N on all of $L^2(\Lambda_L^N)$ is unique, and since H_N commutes with the symmetrization operator S_N, the symmetrization of ψ_N must be equal to ψ_N itself. Therefore, the ground state energy of H_N on all of $L^2(\Lambda_L^N)$ is in fact the same as the ground state energy on the symmetric wave functions $L^2_s(\Lambda_L^N)$.

The construction of the trial state is based on an idea from [19]. We set

$$\psi(x_1,\dots,x_N) = F_1(x_1)F_2(x_1,x_2)\dots F_N(x_1,\dots,x_N),$$

where $F_1 = 1$ and where F_i for $i > 1$ is of the form

$$F_i(x_1, \dots, x_i) = g(t_i), \qquad t_i = \min\big\{|x_i - x_j| : j = 1, \dots, i-1\big\}.$$

In words, F_i is a function that only depends on the distance of x_i to its nearest neighbor of the previous particles $x_1, \dots, x_{i-1}$. Heuristically, one should have in mind to insert the N particles one by one into the system. The function g is defined by

$$g(r) = \begin{cases} f(|x|)/f(b) & : |x| = r \le b, \\ 1 & : |x| > b \end{cases}$$

for some $b = \rho^{-1/3}$ (f denotes the zero energy scattering solution).

We now need to estimate the kinetic and potential energies of our wave function. For the following computations, it will be useful to introduce the notation

$$\varepsilon_{ik}(x_1, \dots, x_N) = \begin{cases} 1 & : \text{for } i = k, \\ -1 & : \text{for } t_i = |x_i - x_k|, \\ 0 & : \text{else.} \end{cases}$$

Furthermore, let us denote in the following by n_i the unit vector

$$n_i = \frac{x_i - x_{j(i)}}{t_i} = \frac{x_i - x_{j(i)}}{|x_i - x_{j(i)}|},$$

where $j(i) \in \{1, \dots, i-1\}$ is chosen such that $|x_i - x_{j(i)}| = t_i$. We then find

$$\frac{1}{\psi}\nabla_k \psi = \frac{1}{\prod_{i=1}^N F_i} \nabla_k \prod_{i=1}^N F_i = \frac{1}{F_i} g'(t_k) n_k + \sum_{i=k+1}^N \frac{1}{F_i} \nabla_k F_i = \sum_{i=1}^N \frac{1}{F_i} \varepsilon_{ik} n_i g'(t_i),$$

which implies after summing over k that

$$\begin{aligned}
&\psi^{-2} \sum_{k=1}^N |\nabla_k \psi|^2 = \sum_{i,j,k=1}^N F_i^{-1} F_j^{-1} \varepsilon_{ik} \varepsilon_{jk} n_i \cdot n_j g'(t_i) g'(t_j) \\
&= \sum_{1 \le k \le i \le N} F_i^{-2} \varepsilon_{ik}^2 g'(t_i)^2 + 2 \sum_{1 \le k \le i < j \le N} F_i^{-1} F_j^{-1} \varepsilon_{ik} \varepsilon_{jk} n_i \cdot n_j g'(t_i) g'(t_j) \\
&\le \sum_{1 \le i \le N} \Big(F_i^{-2} g'(t_i)^2 + \sum_{1 \le k < i \le N} F_i^{-2} \varepsilon_{ik}^2 g'(t_i)^2 \Big) + 2 \sum_{1 \le k \le i < j \le N} F_i^{-1} F_j^{-1} |\varepsilon_{ik} \varepsilon_{jk}| g'(t_i) g'(t_j) \\
&\le 2 \sum_{1 \le i \le N} F_i^{-2} g'(t_i)^2 + 2 \sum_{1 \le k \le i < j \le N} F_i^{-1} F_j^{-1} |\varepsilon_{ik} \varepsilon_{jk}| g'(t_i) g'(t_j).
\end{aligned}$$

The factor 2 for the first sum comes from the observation that, for fixed i, we have $F_i^{-2} g'(t_i)^2 = \sum_{1 \le k < i} F_i^{-2} \varepsilon_{ik}^2 g'(t_i)^2$. The energy of the trial state is thus bounded by

$$\begin{aligned}
\frac{\langle \psi, H_N \psi \rangle}{\|\psi\|^2} \le \sum_{j=1}^N \frac{2 \int \psi^2 F_j^{-2} g'(t_j)^2}{\|\psi\|^2} + \sum_{1 \le i < j \le N} \frac{\int \psi^2 v(x_i - x_j)}{\|\psi\|^2} \\
+ 2 \sum_{1 \le k \le i < j \le N} \frac{\int \psi^2 |\varepsilon_{ik} \varepsilon_{jk}| F_i^{-1} F_j^{-1} g'(t_i) g'(t_j)}{\|\psi\|^2}.
\end{aligned} \tag{4.13}$$

Next, we show that the first two contributions on the r.h.s. in (4.13) can be combined using the scattering equation, once we suitably isolate the dependence on x_i and x_j in the integrands. After that, we show that the third term in (4.13) is an error term.

To combine the first two terms, let us denote by $F_{p,i}$, for $i < p$, the value of F_p if x_i was omitted as possible nearest neighbor, i.e.

$$F_{p,i}(x_1, x_2, \dots, x_p) = g(t_{pi}), \quad t_{p,i} = \min\big\{|x_i - x_j| : j = 1, \dots, i-1, i+1, \dots, p-1\big\}.$$

Then $F_{p,i}$ is certainly independent of x_i and we define analogously $F_{p,ij}$, for $i, j < p$, removing the points x_i, x_j as possible nearest neighbors. We will use these functions to get upper and lower bounds on the factors F_i that appear in both numerator and denominator in the terms in (4.13).

By the monotonicity of the scattering function f and since $0 < f \leq 1$, we have that

$$\begin{aligned} F_{p,i}^2 g^2(|x_p - x_i|) &\leq \big(\min(F_{p,i}, g(|x_p - x_i|)\big)^2 \leq F_{p,i}^2, \\ F_{p,ij}^2 g^2(|x_p - x_i|) g^2(|x_p - x_j|) &\leq \big(\min(F_{p,ij}, g(|x_p - x_i|), g(|x_p - x_j|)\big)^2 \leq F_{p,ij}^2. \end{aligned}$$

To isolate the dependence on the coordinates x_i, x_j, for $i < j$, we then bound

$$F_{i+1}^2 \dots F_{j-1}^2 F_{j+1}^2 \dots F_N^2 \leq F_{i+1,i}^2 \dots F_{j-1,i}^2 F_{j+1,ij}^2 \dots F_{N,ij}^2 \tag{4.14}$$

as well as

$$\begin{aligned} F_i^2 \dots F_N^2 \geq\,& F_{i+1,i}^2 \dots F_{j-1,i}^2 F_{j+1,ij}^2 \dots F_{N,ij}^2 \prod_{r<i} g^2(|x_i - x_r|) \prod_{i<s<j} g^2(|x_s - x_i|) \\ &\times \prod_{t<j} g^2(|x_j - x_t|) \prod_{u>j} g^2(|x_u - x_i|) g^2(|x_u - x_j|) \\ =\,& F_{i+1,i}^2 \dots F_{j-1,i}^2 F_{j+1,ij}^2 \dots F_{N,ij}^2 \prod_{k\neq i, k\neq j} g^2(|x_k - x_i|) \prod_{l\neq j} g^2(|x_l - x_j|). \end{aligned}$$

Using for $0 \leq \epsilon_i \leq 1$ the elementary inequality

$$\prod_i (1 - \epsilon_i) \geq 1 - \sum_i \epsilon_i,$$

which follows easily by induction (*exercise*), we arrive at the lower bound

$$\begin{aligned} F_i^2 \dots F_N^2 \geq\,& F_{i+1,i}^2 \dots F_{j-1,i}^2 F_{j+1,ij}^2 \dots F_{N,ij}^2 \\ &\times \Bigg(1 - \sum_{k\neq i, k\neq j} (1 - g^2(|x_i - x_k|))\Bigg)\Bigg(1 - \sum_{l\neq j} (1 - g^2(|x_j - x_l|))\Bigg). \end{aligned} \tag{4.15}$$

Now, let's use (4.14) to control the numerator in the sum of the first two terms in (4.13) from above. Together with

$$g'(t_j)^2 \leq \sum_{i<j} g'(|x_i - x_j|)^2,$$

we get for fixed $i < j$ that

$$\int \Big(2\psi^2 F_j^{-2} g'(|x_i - x_j|)^2 + \psi^2 v(x_i - x_j)\Big)$$
$$\leq \int \Big(2g'(|x_i - x_j|)^2 + v(x_i - x_j) g^2(|x_i - x_j|)^2\Big) \int F_{i+1,i}^2 \dots F_{j-1,i}^2 F_{j+1,ij}^2 \dots F_{N,ij}^2,$$

where the first factor on the right hand side is equal to

$$2L^3 \int_{B_b} dx \left(|\nabla f_b(x)|^2 + v(x) f_b^2(|x|)^2\right) = 8\pi \mathfrak{a} L^3 (1 - \mathfrak{a}/b)^{-1}.$$

The denominator $\|\psi\|^2$, on the other hand, is bounded from below by

$$\int \psi^2 \geq \int F_{i+1,i}^2 \dots F_{j-1,i}^2 F_{j+1,ij}^2 \dots F_{N,ij}^2$$
$$\times \Big(1 - \sum_{l \neq j} (1 - g^2(|x_j - x_l|))\Big)\Big(1 - \sum_{k \neq i, k \neq j} (1 - g^2(|x_i - x_k|))\Big).$$

Here, we can first integrate out the x_i and x_j variables and then remain with the factor $\int F_{i+1,i}^2 \dots F_{j-1,i}^2 F_{j+1,ij}^2 \dots F_{N,ij}^2$, which cancels the factor from the numerator. With

$$\int_{\Lambda_L} dx_i \Big(1 - \sum_{k \neq i, k \neq j} (1 - g^2(|x_i - x_k|))\Big) = L^3 - (N-2) \int_{\Lambda_L} dx\, (1 - g^2(|x|))$$

and the pointwise bound $f(x) \geq \max\left[0, 1 - \mathfrak{a}|x|^{-1}\right]$ from Problem 4.3, we get

$$\int_{\Lambda_L} dx\, (1 - g^2(|x|)) \leq \frac{4\pi}{3} b^3 + 4\pi \int_{\mathfrak{a}}^b dr\, (r - \mathfrak{a})^2 = \frac{4\pi}{3} b^3 \big(1 - (1 - \mathfrak{a}/b)^3\big).$$

Choosing $b = \rho^{-1/3}$ and putting the previous bounds together, we conclude that

$$\frac{1}{N}\bigg(\sum_{j=1}^N \frac{2\int \psi^2 F_j^{-2} g'(t_j)^2}{\|\psi\|^2} + \sum_{1 \leq i < j \leq N} \frac{\int \psi^2 v(x_i - x_j)}{\|\psi\|^2}\bigg)$$
$$\leq \frac{1}{N} \sum_{j=1}^N \frac{(j-1)}{L^3} \frac{8\pi \mathfrak{a}}{(1 - \mathfrak{a}\rho^{\frac{1}{3}})\big(1 - \frac{4\pi}{3}\big(1 - (1 - \mathfrak{a}\rho^{\frac{1}{3}})^3\big)\big)^2} \leq 4\pi\rho\, \mathfrak{a}\big(1 + O(Y^{\frac{1}{3}})\big). \tag{4.16}$$

This controls the first two terms in (4.13) as desired. To finish the proof, one can proceed similarly for the third term in (4.13), we follow the arguments from [62]. We bound

$$\begin{aligned}
&\sum_{k=1}^{i}\int \psi^2|\varepsilon_{ik}\varepsilon_{jk}|F_i^{-1}F_j^{-1}g'(t_i)g'(t_j)\\
&\leq \sum_{k=1}^{i}\int |\varepsilon_{ik}\varepsilon_{jk}|g(t_i)g(t_j)g'(t_i)g'(t_j)\,dx_idx_j \int F_{i+1,i}^2\dots F_{j-1,i}^2F_{j+1,ij}^2\dots F_{N,ij}^2\\
&\leq 2\sum_{k=1}^{i-1}\bigg(\int_{\Lambda_L} dx_i\, g(|x_i-x_k|)g'(|x_i-x_k|)\bigg)^2\int F_{i+1,i}^2\dots F_{j-1,i}^2F_{j+1,ij}^2\dots F_{N,ij}^2\\
&= 2(i-1)\bigg(\int_{\Lambda_L} dx\, g(|x|)g'(|x|)\bigg)^2\int F_{i+1,i}^2\dots F_{j-1,i}^2F_{j+1,ij}^2\dots F_{N,ij}^2
\end{aligned}$$

for every fixed $i<j$, where in the first step we used once more the upper bound (4.14). The factor $\int F_{i+1,i}^2\dots F_{j-1,i}^2F_{j+1,ij}^2\dots F_{N,ij}^2$ will cancel with the same factor from the denominator, which we bound exactly as in the first step of the proof. Thus, it only remains to control the integral $\int_{\Lambda_L} dx\, g(|x|)g'(|x|)$. Using again Problem 4.3, integration by parts and that $f\leq 1$, we find the simple upper bound

$$\int_{\Lambda_L} dx\, g(|x|)g'(|x|) \leq 4\pi\bigg(\frac{1}{2}b^2-\int_a^b dr\, r(1-\mathfrak{a}/r)^2\bigg)\leq 12\pi\mathfrak{a}\rho^{-1/3}.$$

Inserting this into the previous estimate, summing over i and j and using the same bound for the denominator as in the first step, this yields altogether that

$$\begin{aligned}
&\frac{2}{N}\sum_{1\leq k\leq i<j\leq N}\frac{\int\psi^2|\varepsilon_{ik}\varepsilon_{jk}|F_i^{-1}F_j^{-1}g'(t_i)g'(t_j)}{\|\psi\|^2}\\
&\leq C\frac{N^2}{L^6}\big(\mathfrak{a}\rho^{-1/3}\big)^2\big(1+O(Y^{\frac13})\big)=4\pi\rho\mathfrak{a}\,O(Y^{\frac13})\big(1+O(Y^{\frac13})\big).
\end{aligned}\tag{4.17}$$

Inserting (4.16) and (4.17) into (4.13), this concludes the upper bound. □

4.3 Ground State Energy and BEC in Ultra Dilute Regimes

In this section, we consider the Bose gas in the Gross-Pitaevskii regime with Hamiltonian

$$H_N=\sum_{i=1}^{N}-\Delta_{x_i}+\sum_{1\leq i<j\leq N}N^2V(N(x_i-x_j)).\tag{4.18}$$

This operator is self-adjoint on a suitable dense domain in $L^2_s(\Lambda^N)$ for $\Lambda=\mathbb{T}^3$. As in previous sections, we assume for simplicity that $V\in C_c^\infty(\mathbb{R}^3)$ is radial and non-negative.

The Gross-Pitaevskii regime is characterized by the specific scaling $N^2V(N.)$ of the two-body potential and it is equivalent to what is called an ultra-dilute regime. This is meant in the following sense: by a change of variables (similarly as in Lemma 4.1), studying the spectrum of H_N is equivalent to studying the spectrum of the Hamiltonian

$$H_{N,L} = \sum_{i=1}^{N} -\Delta_{x_i} + \sum_{1\leq i<j\leq N} V(x_i - x_j)$$

in $L^2_s(\Lambda_L^N)$, for the side length $L = N^{1-\kappa}$ with parameter $\kappa = 0$, where

$$\Lambda_L = \mathbb{R}^3/L\mathbb{Z}^3.$$

Notice that the number of particles density $\rho = \rho_N$ of N particles moving in Λ_L for $L = N^{1-\kappa}$, a box of volume $N^{3-3\kappa}$, is equal to $\rho_N = N^{3\kappa-2}$. So, if $\kappa < \frac{2}{3}$, we have that

$$\lim_{N\to\infty} \rho_N = 0.$$

In other words, the limit $N \to \infty$ corresponds to a joint thermodynamic and low-density limit in which the asymptotic number of particles density $\lim_{N\to\infty} \rho_N$ vanishes. Heuristically, one thus considers a system in which the infinite volume limiting theory should resemble a free, non-interacting theory. One might therefore expect that proving BEC in such regimes is simpler compared to the usual thermodynamic limit. This interpretation also suggests that the larger the parameter κ, the faster the density tends to zero as $N \to \infty$ and the closer the theory should be to a non-interacting theory.

What is the simplest scaling regime in which a proof of BEC for the ground state becomes non-trivial? Notice that for $L = N^{1-\kappa}$, $\kappa < 0$, ψ_N denoting the ground state of $H_{N,L}$ and $\varphi_0^{(L)} = L^{-\frac{3}{2}} \in L^2(\Lambda_L)$, one has the trivial upper bound

$$\langle \psi_N, \mathcal{N}_{L,+}\psi_N\rangle \leq L^2\langle \psi_N, H_{N,L}\psi_N\rangle \leq L^2\big\langle (\varphi_0^{(L)})^{\otimes N}, H_{N,L}(\varphi_0^{(L)})^{\otimes N}\big\rangle = N^{1+\kappa}\widehat{v}(0) \ll N,$$

where $\mathcal{N}_+^{(L)} = \sum_{0\neq p\in 2\pi\mathbb{Z}^3/L} a_p^* a_p$ denotes the number of orthogonal excitations in the setting of $L^2_s(\Lambda_L^N)$. Thus, for $\kappa < 0$, complete BEC is trivially true for the ground state (in fact, for every state with energy sufficiently close to the ground state energy). Clearly, the previous argument breaks down at $\kappa = 0$, the Gross-Pitaevskii scaling. The GP regime can thus be viewed as the simplest ultra dilute scaling regime in which correlation effects have a non-trivial impact on the spectrum and the dynamics of the system. Increasing the diluteness parameter $\kappa \geq 0$ further towards $\frac{2}{3}$ interpolates from the Gross-Pitaevskii to the thermodynamic scaling (at density one).

Before discussing the GP scaling in more detail, note also that the mean field systems discussed in Section 3 can be viewed as further simplifications of GP systems. Indeed, in view of (4.18) and the previous discussion, the mean field Hamiltonian in (3.14) describes equivalently a system of N bosons moving in the large volume Λ_N and interacting with the long-range potential $N^{-3}v(N^{-1}.)$. This potential ranges essentially over all of Λ_N and one may think of it as a weak, approximately constant interaction potential. It is therefore not very surprising that a proof of BEC is comparatively simple.

Let us now present some basic results in the GP regime (at the cost of slightly more technical proofs, the following results can also be generalized to ultra-dilute regimes with sufficiently small, but positive $\kappa > 0$). For notational convenience, we consider systems of N bosons moving in $\mathbb{T}^3$ and we analyze the Hamiltonian H_N, defined in (4.18). In terms of the creation and annihilation operators, H_N takes the form

$$H_N = \sum_{p\in\Lambda_+^*} |p|^2 a_p^* a_p + \frac{1}{2N} \sum_{p,q,r\in\Lambda^*} \widehat{V}(r/N) a_{p+r}^* a_{q-r}^* a_p q_q. \tag{4.19}$$

The following result is an analogue of Theorem 3.2.

Theorem 4.3 (Ground State Energy and BEC)**.** *Let $E_N = \inf\sigma(H_N)$ and let ψ_N be a normalized ground state vector. If $\mathfrak{a}$ denotes the scattering length of V, then*

$$E_N = 4\pi\mathfrak{a}N + o(N) \quad \textit{and} \quad \langle\psi_N, \mathcal{N}_+\psi_N\rangle \leq o(N) \tag{4.20}$$

for some error $o(N) \geq 0$ that satisfies $\lim_{N\to\infty} N^{-1}o(N) = 0$.

Remark. *The GP regime has been analyzed in great detail in the past two decades. The first proof of BEC was obtained in [42]. Later, BEC was proved for a larger class of approximate ground states [43, 49] and optimal bounds on the number of excitations were obtained in [4, 7, 48, 14]. Analogous results were proved in parallel in the dynamical setting [23, 24, 26, 25, 53, 3, 13]. Bogoliubov's theory was recently derived in [6] with generalizations to the trapped [50, 15] and the two dimensional setting [18]. For further results on the GP regime, see for instance the review paper [60].*

Proof. We follow [11] and present some key steps of its proof. We refer the interested reader to [11] for the complete details. The proof is a generalization of the arguments in the proof of Lemma 4.1 from the two-body problem to the N-body problem.

Note first that the ground state energy upper bound follows from Theorem 4.2. More precisely, by a simple change of variables, Theorem 4.2 implies that

$$E_N \leq 4\pi\mathfrak{a}N + O(N^{\frac{5}{6}}).$$

So, let's focus on the lower bound and the proof of BEC. Here, we would like to mimic the overall strategy of the proof of Lemma 4.1. Recall that in Lemma 4.1, we first proved BEC based on simple a priori energy bounds, then we deduced the ground state energy lower bound and finally we concluded the upper bound. The key difficulty in the proof of Theorem 4.3 is that simple a priori bounds do not directly imply BEC. We therefore need to find a good replacement for the first step. To this end, let $\zeta \geq 0$ and define

$$\mathcal{N}_{>\zeta} = \sum_{r\in\Lambda^*:|r|>\zeta} a_r^* a_r.$$

Analogously, we define the operators $\mathcal{N}_{\geq\zeta}, \mathcal{N}_{<\zeta}$ and $\mathcal{N}_{\leq\zeta}$; note that $\mathcal{N}_+ = \mathcal{N}_{>0}$. Recalling that $\mathcal{K}_+ = \sum_{r\in\Lambda_+^*} |r|^2 a_r^* a_r$, our key observation is that, although we do not know a priori that $\langle\psi_N, \mathcal{N}_+\psi_N\rangle = o(N)$, we can use the simple form bound

$$\mathcal{N}_{>N^\beta} \leq N^{-2\beta}\mathcal{K}_+ \leq N^{-2\beta} H_N \tag{4.21}$$

to conclude at least that for every $\alpha > 0$, we have that

$$\langle \psi_N, \mathcal{N}_{>N^\alpha} \psi_N \rangle \leq C N^{1-2\alpha} = o(N).$$

In other words, the number of particles of very large momenta (of size greater than N^α) is small compared to the total number N of particles. In view of the strategy of the proof of Lemma 4.1, this suggests to define the low momentum set

$$\mathrm{P_L} = \big\{ p \in \Lambda^* : |p| \leq N^\alpha \big\}. \tag{4.22}$$

We then let $\Pi_\mathrm{L} : L^2(\Lambda^2) \to L^2(\Lambda^2)$ denote the orthogonal projection onto

$$\overline{\mathrm{span}(\varphi_k \otimes \varphi_l : k, l \in \mathrm{P_L})}$$

and set $\Pi_\mathrm{H} = 1 - \Pi_\mathrm{L}$. Substituting the Schur complement identity

$$\begin{aligned} V_N &= (1 + N^{-1}\eta^*)\big(-\Delta_{x_1} - \Delta_{x_2} + N^{-1}\Pi_\mathrm{L} V_\mathrm{ren} \Pi_\mathrm{L} + \Pi_\mathrm{H} V_N \Pi_\mathrm{H} \big)(1 + N^{-1}\eta) \\ &\quad + \Delta_{x_1} + \Delta_{x_2}, \\ &= \Pi_\mathrm{L} V_\mathrm{ren} \Pi_\mathrm{L} + N^{-1}\eta^*(-\Delta_{x_1} - \Delta_{x_2}) + (-\Delta_{x_1} - \Delta_{x_2}) N^{-1}\eta \\ &\quad + N^{-1}\eta^*(-\Delta_{x_1} - \Delta_{x_2}) N^{-1}\eta + (1 + N^{-1}\eta^*)\Pi_\mathrm{H} V_N \Pi_\mathrm{H}(1 + N^{-1}\eta), \end{aligned}$$

where we set $V_N = N^2 V(N(x_1 - x_2))$ as well as

$$\begin{aligned} \eta &= N\, \Pi_\mathrm{H} \big[\Pi_\mathrm{H}(-\Delta_{x_1} - \Delta_{x_2} + V_N)\Pi_\mathrm{H} \big]^{-1} \Pi_\mathrm{H} V_N \Pi_\mathrm{L}, \\ V_\mathrm{ren} &= N\big(V_N - V_N \Pi_\mathrm{H} \big[\Pi_\mathrm{H}(-\Delta_{x_1} - \Delta_{x_2} + V_N)\Pi_\mathrm{H} \big]^{-1} \Pi_\mathrm{H} V_N \big), \end{aligned}$$

into H_N leads to the identity (*exercise*)

$$\begin{aligned} H_N = \sum_{r \in \Lambda_+^*} |r|^2 c_r^* c_r &+ \frac{1}{2N} \sum_{\substack{p,q,r \in \Lambda^* : \\ p,q,p+r,q-r \in \mathrm{P_L}}} \langle \varphi_{p+r} \otimes \varphi_{q-r}, V_\mathrm{ren} \varphi_p \otimes \varphi_q \rangle a_{p+r}^* a_{q-r}^* a_p a_q \\ &+ \frac{1}{2N} \sum_{p,q,r \in \Lambda^*} \big\langle \varphi_{p+r} \otimes \varphi_{q-r}, \big(1 + \frac{\eta^*}{N}\big) \Pi_\mathrm{H} V_N \Pi_\mathrm{H} \big(1 + \frac{\eta}{N}\big) \varphi_p \otimes \varphi_q \big\rangle a_{p+r}^* a_{q-r}^* a_p a_q - R_N. \end{aligned} \tag{4.23}$$

Here, we recall that $\Lambda_+^* = \Lambda^* \setminus \{0\}$ and we introduced the operators

$$\begin{aligned} c_r &= a_r + \frac{1}{N} \sum_{(p,q) \in \mathrm{P_L^2}} \langle \varphi_{p+q-r} \otimes \varphi_r, \eta\, \varphi_p \otimes \varphi_q \rangle a_{p+q-r}^* a_p a_q \quad (\forall\, r \in \Lambda^*), \\ R_N &= \frac{1}{N^2} \sum_{r,p,q,s,t \in \Lambda^*} |r|^2 \langle \eta\, \varphi_p \otimes \varphi_q, \varphi_{p+q-r} \otimes \varphi_r \rangle \langle \varphi_{s+t-r} \otimes \varphi_r, \eta\, \varphi_s \otimes \varphi_t \rangle \\ &\qquad \times a_p^* a_q^* a_{s+t-r}^* a_{p+q-r} a_s a_t. \end{aligned} \tag{4.24}$$

By the positivity of $V_N \geq 0$, we can lower bound the r.h.s. in (4.23) by

$$H_N \geq \sum_{r\in\Lambda_+^*} |r|^2 c_r^* c_r + \frac{1}{2N} \sum_{\substack{p,q,r\in\Lambda^*:\\ p,q,p+r,q-r\in \mathrm{P_L}}} \langle \varphi_{p+r}\otimes\varphi_{q-r}, V_{\mathrm{ren}}\varphi_p\otimes\varphi_q\rangle a_{p+r}^* a_{q-r}^* a_p a_q - R_N. \tag{4.25}$$

To control the r.h.s. in (4.25) further from below, we use several bounds that are proved in detail in [11] (see also [17]): a careful and elementary analysis shows that

$$\begin{aligned} \big|\langle \varphi_{k_1}\otimes\varphi_{k_2}, V_{\mathrm{ren}}\varphi_{k_3}\otimes\varphi_{k_4}\rangle\big| &\leq C,\\ \big|\langle \varphi_{k_1}\otimes\varphi_{k_2}, V_{\mathrm{ren}}\varphi_{k_3}\otimes\varphi_{k_4}\rangle - 8\pi\mathfrak{a}\big| &\leq \frac{C}{N}\Big(N^\alpha + \sum_{i=1}^4 N^{-\alpha}|k_i|^2\Big),\\ \big|\langle \varphi_{k_1}\otimes\varphi_{k_2}, \eta\,\varphi_{k_3}\otimes\varphi_{k_4}\rangle\big| &\leq \frac{C\,\delta_{k_1+k_2,k_3+k_4}}{|k_1|^2+|k_2|^2}\mathbf{1}_{(\mathrm{P_L^2})^c}((k_1,k_2))\mathbf{1}_{\mathrm{P_L^2}}((k_3,k_4)) \end{aligned} \tag{4.26}$$

for some $C>0$ and for all $k_1,k_2,k_3,k_4\in\Lambda^*$ that satisfy $k_1+k_2=k_3+k_4$. On the other hand, it is a straightforward observation (*exercise*) that V_{ren} is a translation invariant operator so that $\langle \varphi_{k_1}\otimes\varphi_{k_2}, V_{\mathrm{ren}}\varphi_{k_3}\otimes\varphi_{k_4}\rangle = 0$ if $k_1+k_2\neq k_3+k_4$.

Now, let's use the bounds in (4.26) to control the r.h.s. in (4.25) further. First of all, we notice that the leading order energy contribution is hidden in the renormalized potential energy term. This follows from the mean field type estimate

$$\begin{aligned} &\frac{1}{2N} \sum_{\substack{p,q,r\in\Lambda^*:\\ p,q,p+r,q-r\in \mathrm{P_L}}} \langle \varphi_{p+r}\otimes\varphi_{q-r}, V_{\mathrm{ren}}\varphi_p\otimes\varphi_q\rangle a_{p+r}^* a_{q-r}^* a_p a_q\\ &\geq \frac{4\pi\mathfrak{a}}{N} \sum_{\substack{p,q,r\in\Lambda^*:\\ p,q,p+r,q-r\in \mathrm{P_L}}} a_{p+r}^* a_{q-r}^* a_p a_q - CN^{\alpha-2}|\mathrm{P_L}|\mathcal{N}_{\leq 2N^\alpha}^2\\ &\geq \frac{4\pi\mathfrak{a}}{N}\Big(\sum_{q\in\mathrm{P_L}} a_q^* a_q\Big)^*\Big(\sum_{q\in\mathrm{P_L}} a_q^* a_q\Big) - \frac{4\pi\mathfrak{a}}{N}\sum_{\substack{p,r\in\Lambda^*:\\ p,p+r\in\mathrm{P_L}}} a_{p+r}^* a_{p+r} - CN^{4\alpha}\\ &\geq \frac{4\pi\mathfrak{a}}{N}\big(N-\mathcal{N}_{>N^\alpha}\big)^2 - CN^{4\alpha} \geq 4\pi\mathfrak{a}N - CN^{-2\alpha}\mathcal{K}_+ - CN^{4\alpha}. \end{aligned} \tag{4.27}$$

Similarly, we can control the renormalized kinetic energy. Recalling (4.24) and setting

$$d_r = \frac{N^\kappa}{N}\sum_{(p,q)\in\mathrm{P_L^2}} \langle \varphi_{p+q-r}\otimes\varphi_r, \eta\,\varphi_p\otimes\varphi_q\rangle a_{p+q-r}^* a_p a_q,$$

so that $c_r = a_r + d_r$, we lower bound

$$\begin{aligned}
&\sum_{r\in\Lambda_+^*} |r|^2 c_r^* c_r - 4\pi^2\big(\mathcal{N}_{<N^\beta} - a_0^* a_0\big)\\
&\geq \sum_{r\in\Lambda_+^*:0<|r|<N^\beta} 4\pi^2 c_r^* c_r - \sum_{r\in\Lambda_+^*:0<|r|<N^\beta} 4\pi^2 a_r^* a_r\\
&= \sum_{r\in\Lambda_+^*:0<|r|<N^\beta} 4\pi^2\big(d_r^* a_r + a_r^* d_r + d_r^* d_r\big)\\
&\geq \frac{4\pi^2}{N} \sum_{p,q,r\in\Lambda^*:0<|r|<N^\beta} \langle \varphi_{p+q-r}\otimes\varphi_r, \eta\,\varphi_p\otimes\varphi_q\rangle a_r^* a_{p+q-r}^* a_p a_q + \text{h.c.},
\end{aligned}$$

for some $\beta < \alpha$. Together with (4.26) and Cauchy-Schwarz, we obtain for $\xi \in L^2_s(\Lambda^N)$

$$\begin{aligned}
&\left|\frac{1}{N} \sum_{p,q,r\in\Lambda^*:0<|r|<N^\beta} \langle \varphi_{p+q-r}\otimes\varphi_r, \eta\,\varphi_p\otimes\varphi_q\rangle \langle \xi a_r^* a_{p+q-r}^* a_p a_q \xi\rangle\right|\\
&\quad\leq \frac{C}{N^{1+2\alpha}} \sum_{\substack{(p,q,r)\in P_L^3:\\ 0<|r|<N^\beta,\,|p|>\frac{1}{3}N^\alpha,\,p+q-r\in \mathrm{P}_\mathrm{L}^c}} \|a_r a_{p+q-r}\xi\|\|a_p a_q \xi\| \qquad (4.28)\\
&\quad\leq CN^{\frac{3}{2}\beta-\frac{1}{2}\alpha}\langle \xi, \mathcal{N}_{>\frac{1}{3}N^\alpha}\xi\rangle \leq CN^{-\alpha}\langle\xi,\mathcal{K}_+\xi\rangle
\end{aligned}$$

Notice that due to the constraint $p + q - r \in \mathrm{P}_\mathrm{L}^c$ and the condition $|r| < N^\beta$ for $\beta < \alpha$, at least one of the momenta p and q has to be larger than $\frac{1}{3}N^\alpha$ for large N.

Now, combining (4.25), (4.27) and (4.28) (for the choice $\beta = \frac{\alpha}{2}$, $\alpha = \frac{1}{5}$) with the fact that $\langle\psi_N, \mathcal{K}_+\psi_N\rangle \leq CN$ for the ground state ψ_N of H_N, we obtain the lower bound

$$\langle\psi_N, H_N\psi_N\rangle \geq 4\pi\mathfrak{a}N + c\,\langle\psi_N, \mathcal{N}_+\psi_N\rangle - \langle\psi_N, R_N\psi_N\rangle - CN^{\frac{4}{5}}.$$

for suitable $C, c > 0$. Using similar arguments as in (4.27) and (4.28), one can finally show that $\langle\psi_N, R_N\psi_N\rangle = o(N)$ (see [11] for the details) so that

$$4\pi\mathfrak{a}N + o(N) \geq \langle\psi_N, H_N\psi_N\rangle \geq 4\pi\mathfrak{a}N + c\,\langle\psi_N, \mathcal{N}_+\psi_N\rangle + o(N).$$

This proves (4.20) and finishes the proof of Theorem 4.3. □

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