The mathematics of dilute quantum gases

1. Introduction

- Quantum mechanical description of N bosonic/fermionic particles in a box
- Thermodynamic limit
- Sobolev spaces and Sobolev inequalities
- Hilbert spaces, (unbounded) operators, extensions of operators, quadratic forms, spectral theorem and variational principle for the eigenvalues

1.) Quantum mechanical description of N particles in a box

The dynamics of N quantum particles in the box $[0,L]^d \subset \mathbb{R}^d$ is descripted by the time-dependent Schrödinger equation

$$i\dot{\Psi}_t = H_N \Psi_t \quad \text{with initial condition } \Psi_{t=0} = \Psi_0 \qquad (1)$$

and Hamilton operator (or Hamiltonian)

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \le i < j \le N} V(x_i - x_j). \qquad (2)$$

The function $V: \mathbb{R}^d \to \mathbb{R}$ denotes the interaction potential. In the cases we are interested in V will be nonnegative, radial and of compact support.

The wave functions are complex-valued and depend on the N particle coordinates $x_1 \dots x_N \in [0,L]^d$. By $-\Delta_i$ we denote the Laplacian acting on x_i. Depending on the situation, we will choose it with either Dirichlet, Neumann or periodic boundary

conditions. If the initial condition $\Psi_0 \in L^2([0,L]^{dN})$ obeys
$$\int_{[0,L]^{dN}} |\Psi_0(x_1 \dots x_N)|^2 d(x_1 \dots x_N) = 1 \,,$$
then this property is also shared by $\Psi_t(x_1 \dots x_N)$. In quantum mechanics

$$\rho_\Psi(x_1 \dots x_N) = |\Psi(x_1, \dots, x_N)|^2 \tag{3}$$

has the interpretation of an N-particle probability distribution. If one is interested in the N-particle probability distribution of the momenta of the particles one has to consider (only in case of periodic BC's)

$$\rho_{\hat{\Psi}}(p_1, \dots, p_N) = |\hat{\Psi}(p_1, \dots, p_N)|^2. \tag{4}$$

Let us denote the $L^2([0,L]^{dN})$ scalar product by

$$\langle f, g \rangle = \int_{[0,L]^{dN}} \overline{f(x_1 \dots x_N)}\, g(x_1 \dots x_N)\, d(x_1 \dots x_N) \tag{5}$$

and recall that $L^2([0,L]^{dN})$ with this scalar product is a Hilbert space. The Hamiltonian is an unbounded self-adjoint operator on this Hilbert space (we discuss later what this exactly means) and has a complete set of eigenvectors, that is,

$$H_N = \sum_{i=0}^{\infty} E_i \, |\Psi_i \rangle\langle \Psi_i|, \qquad (6)$$

where $|\Psi_i\rangle\langle\Psi_i|$ denotes the orthogonal projection on the vector Ψ_i.

The eigenvectors Ψ_i are stationary solutions of (1) in the sense that if $\Psi_{t=0} = \Psi_i$, then $\Psi(t) = e^{-iE_i t}\Psi_i$. Of particular interest are the lowest eigenvalue E_0 of H_N and the related eigenvector Ψ_0 because it turns out that quantum system at very low temperatures are with good approximation descripted by Ψ_0. The eigenvalue E_0 is interpreted as the energy of the system. The energy of a general wave function $\Psi \in L^2([0,L]^{dN})$ with $\|\Psi\| = \langle \Psi, \Psi\rangle^{1/2} = 1$ is given by

$$\mathcal{E}(\Psi) = \langle \Psi, H_N \Psi \rangle. \qquad (7)$$

That is, the wave function Ψ_0 has the lowest possible energy.

The eigenvalues and eigenvectors of H_N are solutions of the time-independent Schrödinger equation

$$H_N \Psi = E \Psi. \tag{8}$$

If we have a closer look at the Hamiltonian H_N in (2) we see that all particle coordinates appear in a symmetric way. That is, if we interchange two coordinates H_N stays the same. Assume for the moment that Ψ is a solution of (8) and that the eigenvalue E is simple. Define by P_{ij} the operator on $L^2([0,L]^{dN})$ that interchanges x_i and x_j, that is,

$$P_{ij} \Psi(x_1 .. x_i .. x_j .. x_N) = \Psi(x_1 .. x_j .. x_i .. x_N). \tag{9}$$

When we apply P_{ij} to (8) we see that $P_{ij}\Psi$ is also a solution of (8). Since the eigenvalue E is simple and $[P_{ij}, H_N] = 0$ we know that Ψ is also an eigenfunction of P_{ij}, that is, $P_{ij}\Psi = c\Psi$ with $|c| = 1$ because $\langle P_{ij}\phi, P_{ij}\phi\rangle = \langle\phi,\phi\rangle$ for all $\phi \in L^2([0,L]^{dN})$. Since $P_{ij}^2 = 1$ we conclude $c = \pm 1$. Note that the same argument does not work if E is degenerate. Note also that if $P_{ij}\Psi = \Psi$ and $P_{ik}\Psi = \Psi$ for pairwise unequal i,j,k, then $P_{jk}\Psi = \Psi$.

In nature we encounter only two sorts of particles, those described by totally symmetric wave functions ($\Psi(x_1 .. x_i .. x_j .. x_N) = \Psi(x_1 .. x_j .. x_i .. x_N) \ \forall ij$) called bosons and those described by a totally anti-symmetric wave function ($\Psi(x_1 .. x_i .. x_j .. x_N) = (-1)\, \Psi(x_1 .. x_j .. x_i .. x_N) \ \forall ij$) called fermions. Note that these considerations only apply to identical particles because otherwise the particle coordinates $x_1 \cdots x_N$ would not appear in a symmetric way in the Hamiltonian. Two non-interacting particles with mass m_1 and m_2 would e.g. be descripted by the Hamiltonian

$$H_{m_1 m_2} = -\frac{\Delta}{2m_1} - \frac{\Delta}{2m_2} \,. \tag{10}$$

Symmetric / antisymmetric wave functions form a linear closed subspace of $L^2([0,L]^{dN})$ that is invariant under the time evolution w.r.t. (1).

From a more algebraic point of view

$$L^2([0,L]^{dN}) = \bigotimes_{j=1}^{N} L^2([0,L]^d). \tag{11}$$

Let $L^2_{s/a}([0,L]^{dN})$ be the subspace of symmetric/antisymmetric functions in $L^2([0,L]^{dN})$ and denote by $\otimes_{s/a}$ the symmetric/antisymmetric tensor product. We then have

$$L^2_{s/a}([0,L]^{dN}) = \bigotimes_{s/a,\, j=1}^{N} L^2([0,L]^d). \quad (12)$$

<u>Example (two particle wave functions)</u>: Let

$\phi_1, \phi_2 \in L^2([0,L]^3)$ with $\|\phi_1\| = 1 = \|\phi_2\|$. Then

$$\Psi_{s/a}(x_1,x_2) = \frac{1}{\sqrt{2}}\Big(\phi_1(x_1)\,\phi_2(x_2) \pm \phi_2(x_1)\,\phi_1(x_2)\Big) \in L^2_{s/a}\big([0,L]^{2d}\big)$$

$$\Big[\ \Psi_{s/a} = \frac{1}{\sqrt{2}}\big(\phi_1 \otimes \phi_2 \pm \phi_2 \otimes \phi_1\big)\ \Big].$$ fermionic/bosonic 2-particle wave function

and $\|\Psi_{s/a}\| = \langle \Psi_{s,a}, \Psi_{s,a}\rangle^{1/2} = 1$.

Examples for fermions: electrons, protons, neutrons, atoms with an odd number of neutrons in the nucleus as e.g. ^{3}He, atomic nuclei where the number of neutrons plus protons is odd.

Examples for bosons: photons (light quanta), atoms with an even number of neutrons in the nucleus as e.g. ^4He, atomic nuclei where the number of neutrons plus protons is even.

2.) The thermodynamic limit

In a sample of matter of the size of $1\,cm^3$, the number of particles in the system is comparable to the Avogadro number $N_a \sim 10^{23}$. In order to describe the bulk behavior of such a system, one usually considers the thermodynamic limit, that is, the limit $N \to \infty$, $L \to \infty$ with $\rho = N/L^d$ fixed. One quantity we are going to consider is the ground state energy per unit volume defined by

in either bosonic or fermionic subspace

$$e_0(\rho) = \lim_{\substack{N\to\infty \\ L\to\infty \\ N/L^3=\rho}} \frac{E_0(N,L)}{L^3}, \qquad (13)$$

where $E_0(N,L)$ denotes the lowest eigenvalue of (2). The existence of the thermodynamic limit for $E_0(N,L)$ and its independence of the boundary conditions can be shown with standard methods, see e.g.

[1,2]. Here we do not discuss these issues.

References:

[1] D.W. Robinson, "The thermodynamic pressure in quantum statistical mechanics", Springer lecture notes in Physics, Vol. 9 (1971).

[2] D. Ruelle, "Statistical mechanics. Rigorous results", World Scientific (1999).

3. Sobolev spaces and Sobolev inequalities

Let $\Omega \subseteq \mathbb{R}^d$ be a nonempty open set and define for $m \in \mathbb{N}_0$, $1 \le p \le \infty$ the Sobolev norms

$$\|f\|_{H^{m,p}} = \Big(\sum_{1 \le |\alpha| \le m} \|D^\alpha f\|_{L^p(\Omega)} \Big)^{1/p} \quad \text{if } 1 \le p < \infty,$$

$$\|f\|_{H^{m,\infty}} = \max_{0 \le |\alpha| \le m} \|D^\alpha f\|_{L^\infty(\Omega)}. \qquad (14)$$

Here $D^\alpha = D_1^{\alpha_1} \cdots D_d^{\alpha_d}$ with $\alpha \in \mathbb{N}_0^d$ and $|\alpha| = \alpha_1 + \dots + \alpha_d$.

We define the Sobolev spaces

$$H^{m,p}(\Omega) = \underbrace{\overline{\mathcal{C}^\infty(\Omega)}^{H^{m,p}}}_{\hookrightarrow\ \Omega \text{ bounded}} \quad \text{and} \quad H_0^{m,p}(\Omega) = \overline{\mathcal{C}_c^\infty(\Omega)}^{H_{1}p}. \qquad (15)$$

It can be shown, see e.g. [3], that the space $H^{m,p}(\Omega)$ consists for $1 \leq p < \infty$ of functions that have m weak derivatives in $L^p(\Omega)$. Let us quickly recall what this means in the case $H^{1,p}(\Omega)$ in some more detail. A function $f \in L^p(\Omega)$ is said to have one weak derivative in $L^p(\Omega)$ if there exists a function $g \in L^p(\Omega)$ s.t.

$$-\int_\Omega f(x)\, \nabla\varphi(x)\, dx = \int_\Omega g(x)\, \varphi(x)\, dx \qquad (16)$$

holds for all test functions $\varphi \in C_c^\infty(\Omega) = \{ f \in C^\infty(\Omega) \mid \mathrm{supp}(f) \subset\subset \Omega \}$. In this case we say that g is the weak gradient of f and write $\nabla f = g$.

The spaces $H_0^{m,p}$ consist of functions with m weak derivatives s.t. its first $m-1$ derivatives obey zero boundary conditions in a weak sense. In the case of a function $f \in H_0^{1,p}(\Omega)$ with $\partial\Omega \in C^1$ this means that the restriction of f to the boundary can be defined and yields a function in $L^p(\partial\Omega)$. More information on this can be found in [4].

Consider the cone $\{x \in \mathbb{R}^d \mid x \neq 0,\ 0 < x_d < |x| \cos \Theta\}$.
This is a cone with opening angle Θ and vertex at the origin. Let $K_{\Theta,r}$ be the finite cone that is obtained by intersecting the above cone with a ball of radius r centered at the origin. A domain $\Omega \subset \mathbb{R}^d$ is said to have the cone property if there exists a fixed finite cone $K_{\Theta,r}$ such that for every $x \in \Omega$ there is a finite cone K_x congruent to $K_{\Theta,r}$, that is contained in Ω and whose vertex is x.

<u>Sobolev inequalities for $H^{1,p}(\Omega)$</u>: Let $\Omega \subset \mathbb{R}^d$ (bounded) be a domain that has the cone property for some Θ and r. Let $1 \leq p < d$ and $f \in H^{1,p}(\Omega)$. Then $f \in L^q(\Omega)$, $q \in [1, p^*]$, $p^* = \dfrac{dp}{d-p}$ and we have

$$\|f\|_{L^{p^*}(\Omega)} \leq C \|f\|_{H^{1,p}(\Omega)} \qquad (17)$$

with a constant C depending on p, d and Ω.
(See e.g. [4] or [5].)

<u>Poincaré inequality for $H^{1,p}_0(\Omega)$</u>: Let $\Omega \subset \mathbb{R}^d$ (Ω bounded) be a domain that has the cone property for some Θ and r. Let $1 \leq p < d$, $f \in H^{1,p}(\Omega)$ and $p^* = \dfrac{dp}{d-p}$. Then we have

the estimate $\|f\|_{L^q(\Omega)} \leq C \|\nabla f\|_{L^p(\Omega)}$

for each $q \in [1, p^*]$ with a constant C depending only on p, q, d and Ω.

<u>Sobolev inequality in $\mathbb{R}^d$, $d \geq 3$</u>

Let $f : \mathbb{R}^d \to \mathbb{C}$ be a measurable function with $\nabla f \in L^2(\mathbb{R}^d)$ and such that the set $\{|f(x)| > a\}$ has finite measure for any $a > 0$. Then $f \in L^q(\mathbb{R}^d)$ with $q = \frac{2d}{d-2}$ and the inequality

$$\|\nabla f\|^2_{L^2(\mathbb{R}^d)} \geq S_d \|f\|^2_{L^q(\mathbb{R}^d)} \qquad (18)$$

holds for some (explicitly known) constant $S_d > 0$.
(See [5], Theorem 8.3)

<u>References:</u>

[3] A. Adams, J.F. Fournier, "Sobolev spaces", Academic press (2003).
(The result can be found in Chapter 3)

[4] L.C. Evans, "Partial differential equations", Americ. Math. Soc. (1997).

(Chapter 5 contains an introduction to Sobolev spaces, in Chapter 5.5 boundary values are discussed.)

[5] E.H. Lieb, M. Loss, "Analysis", Americ. Math. Soc. (2001)

4.1) Hilbert spaces and (unbounded) operators

Definition (Hilbert space): A Hilbert space $\mathcal{H}$ is a vector space with a scalar product $\langle \cdot, \cdot \rangle$ such that $\|\phi\| = \langle \phi, \phi \rangle^{1/2}$ defines a norm in which $\mathcal{H}$ is complete.

From now on $\mathcal{H}$ will be a $\mathbb{C}$-vector space that is separable, that is, it contains a countable dense set. Then:

- Every Hilbert space has an orthonormal basis $S = \{\phi_\alpha\}_{\alpha=1}^{\infty}$ s.t. for each $\phi \in \mathcal{H}$ one has

$$\phi = \sum_{\alpha=1}^{\infty} \langle \phi_\alpha, \phi \rangle \phi_\alpha \qquad \text{(norm convergent sum)}$$

$$\text{and} \quad \|\phi\|^2 = \sum_{\alpha=1}^{\infty} |\langle \phi_\alpha, \phi \rangle|^2 . \tag{19}$$

- (Riesz representation theorem): To any linear functional $\ell : \mathcal{H} \to \mathbb{C}$ with $|\ell(\phi)| \leq C \|\phi\|$ for all $\phi \in \mathcal{H}$ there is a unique vector $\psi \in \mathcal{H}$ with $\ell(\phi) = \langle \psi, \phi \rangle$ for all $\phi \in \mathcal{H}$.

Example: $L^2(\mathbb{R}^d)$ with its natural scalar product is a Hilbert space. The same is true for $H^{k,2}$ (Ex: What is the scalar product?)

Definition (Operators): By an operator (or more precisely densely defined operator) T on a Hilbert space $\mathcal{H}$, we mean a linear map $T: D(T) \to \mathcal{H}$ defined on a dense subspace $D(T) \subset \mathcal{H}$. Dense refers to the fact that $\overline{D(T)}^{\|\cdot\|} = \mathcal{H}$. If $D(T) = \mathcal{H}$ and there exists a constant C s.t. $\|T\phi\| \leq C\|\phi\|$ for all $\phi \in \mathcal{H}$ we say that T is bounded.

Example: The Laplacian can be defined on $C_c^\infty(\mathbb{R}^d)$, which is a dense subset of $L^2(\mathbb{R}^d)$. We cannot define $\Delta\phi$ for all $\phi \in L^2(\mathbb{R}^d)$, and accordingly Δ is not bounded. The operator $\mathcal{M}_x f(x) = x f(x)$ on $L^2([0,1])$ is a bounded operator.

Definition (Extention of an operator): If S and T are two operators such that $D(S) \subseteq D(T)$ and $S\phi = T\phi$ for all $\phi \in D(S)$ then we write $S \subset T$ and say that T is an extension of S.

Definition (Symmetric operator): We say that T is a symmetric operator if $\langle \psi, T\phi \rangle = \langle T\psi, \phi \rangle$ for all $\phi, \psi \in D(T)$.

Example: Integration by parts shows

$$\int_{\mathbb{R}^d} \overline{\psi(x)} \Delta \phi(x)\, dx = \int_{\mathbb{R}^d} \overline{(\Delta \psi(x))}\, \phi(x)\, dx \quad \forall\, \psi, \phi \in C_c^\infty(\mathbb{R}^d).$$

Also $\langle \psi, M_x \phi \rangle = \langle M_x \psi, \phi \rangle$ for all $\psi, \phi \in L^2([0,1])$.

Definition (Adjoint of an operator): If T is an operator we define its adjoint T^* to be the linear map $T^* : D(T^*) \to \mathcal{H}$ defined on the domain

$$D(T^*) = \left\{ \phi \in \mathcal{H} \;\middle|\; \sup_{\psi \in D(T),\, \|\psi\| = 1} |\langle \phi, T\psi \rangle| < +\infty \right\}$$

and with $T^*\phi$ defined by

$$\langle T^*\phi, \psi \rangle = \langle \phi, T\psi \rangle$$

for all $\psi \in D(T)$. If $D(T^*)$ is dense in $\mathcal{H}$ then T^* is an operator.

<u>Definition (Self-adjoint operator)</u>: An operator T is called self-adjoint if $D(T) = D(T^*)$ and if T is symmetric.

<u>Example</u>: Δ with $D(\Delta) = \mathcal{C}_c^\infty(\mathbb{R}^d)$ is not self-adjoint but Δ with $D(\Delta) = H^{2,2}(\mathbb{R}^d)$ is self-adjoint.

Assume that $D(\Delta) = \mathcal{C}_c^\infty(\mathbb{R}^d)$. One easily checks that $f(x) = e^{-x^2} \in D(\Delta^*)$ but $f \notin \mathcal{C}_c^\infty(\mathbb{R}^d)$. This proves the first claim. The second claim can be proved with techniques that we introduce later in the introduction.

The value of self-adjoint operators is that one can prove a spectral theorem for them which is not true for symmetric operators.

4.2) Semi-bounded operators and quadratic forms

Definition (positive operator): An operator $(T, D(T))$ is said to be positive if $\langle \phi, T\phi \rangle \geq 0$ for all $\phi \in D(T)$.

Definition (operator ordering): If $(S, D(S))$ and $(T, D(T))$ are two operators s.t. $D(S) \cap D(T)$ is dense in $\mathcal{H}$ and $T - S \geq 0$ on that subspace we write $S \leq T$.

Definition (Semi-bounded operators): An operator $(T, D(T))$ is said to be semi-bounded below if there exists a $c > 0$ s.t. $T \geq -c\mathbb{1}$.

Definition (Quadratic forms): A quadratic form q is a map $q : Q(q) \times Q(q) \to \mathbb{C}$, where $Q(q) \subset \mathcal{H}$ is a dense linear subspace, which is sesquilinear:

$$q(\lambda\phi_1 + \mu\phi_2, \psi) = \bar{\lambda}\, q(\phi_1, \psi) + \bar{\mu}\, q(\phi_2, \psi)$$

$$q(\phi, \lambda\psi_1 + \mu\psi_2) = \lambda\, q(\phi, \psi_1) + \mu\, q(\phi, \psi_2).$$

A quadratic form is said to be positive if $q(\phi,\phi) \geq 0$ for all $\phi \in Q(q)$ and it is bounded from below if $q(\phi,\phi) \geq -c\|\phi\|^2$ for some $c \in \mathbb{R}$.

We will, by a slight abuse of notation, write

$$q(\phi,\phi) = q(\phi).$$

Exercise: Show that if $(q, Q(q))$ is positive, then

$$|q(\psi,\phi)| \leq q(\psi,\psi)^{1/2} q(\phi,\phi)^{1/2}.$$

(Cauchy-Schwarz inequality)

4.3 Extensions of operators and closed quadratic forms

Definition (Closed operator): An operator T on a Hilbert space $\mathcal{H}$ is said to be closed if its graph

$$\mathcal{G}(T) = \{ (\phi, T\phi) \in \mathcal{H} \oplus \mathcal{H} \mid \phi \in D(T) \}$$

is closed in the Hilbert space $\mathcal{H} \oplus \mathcal{H}$. It is said to be closable if it has a closed extension. Every closable operator has a smallest closed extension called its closure and denoted by $\overline{T}$.

Theorem (Closability of symmetric operators): Let $(T, D(T))$ be a symmetric operator on $\mathcal{H}$. Then T is closable and the graph of its closure is given by the closure of its graph.

Proof: Define R with $D(R) = \{\psi \mid (\psi, \phi) \in \overline{\mathcal{G}(T)}$ for some $\phi \in \mathcal{H}\}$ by $R\psi = \phi$. To see that ϕ is unique we assume $\psi_n^1 \to \psi \leftarrow \psi_n^2$ with $T\psi_n^1 \to \phi_1$ and $T\psi_n^2 \to \phi_2$. Let $v \in D(T)$ and consider

$$\langle v, \phi_1 - \phi_2 \rangle = \lim_{n\to\infty} \langle v, T(\psi_n^1 - \psi_n^2) \rangle = \lim_{n\to\infty} \langle Tv, \psi_n^1 - \psi_n^2 \rangle = 0.$$

Since $D(T)$ is dense in $\mathcal{H}$ we conclude that $\phi_1 = \phi_2$ and that $(R, D(R))$ is well-defined. In particular $\mathcal{G}(R) = \overline{\mathcal{G}(T)}$. One easily checks that R is the smallest closed extension of T. ∎

Definition (Closed quadratic form): A quadratic form $(q, Q(q))$ satisfying the lower bound $q(\phi) \geq -\alpha \|\phi\|^2$ for some $\alpha \geq 0$ is said to be closed if the domain $Q(q)$ equipped with the norm

$$\|\phi\|_q = \sqrt{(\alpha+1)\|\phi\|^2 + q(\phi)}$$

is a Banach space.

Example: Let $q(\psi, \varphi) = \int_{\mathbb{R}^d} \overline{\nabla\psi}(x) \nabla\phi(x) dx$ be defined on $D(q) = H^1(\mathbb{R}^d)$ [Here and in the following we use the notation $H^{n,2}(\Omega) = H^n(\Omega)$.]. We have $q(\psi, \psi) \geq 0$ and $\|\phi\|_q = \sqrt{\|\phi\|^2 + \|\nabla\phi\|^2}$ is nothing but the $H^1(\mathbb{R}^d)$-norm defined in Section 3. Accordingly, $(q, Q(q))$ is a closed quadratic form.

Theorem (Friedrichs extension): Let $(T, D(T))$ be a symmetric positive operator and let $q(\varphi,\psi) = \langle \varphi, T\psi \rangle$ for $\varphi,\psi \in D(T)$. Then q is a closable quadratic form and its closure $\hat{q}$ is the quadratic form of a unique self-adjoint operator $(\hat{T}, D(\hat{T}))$ with domain $Q(\hat{q}) = \overline{D(\hat{T})}^{\|\cdot\|_{\hat{q}}}$. Furthermore, $\hat{T}$ is the only self-adjoint extension of T whose domain is contained in the form domain of $\hat{q}$.

Remark 1: We call $Q(\hat{T}) = Q(\hat{q})$ the form domain of $\hat{T}$.

Remark 2: In general the Friedrichs extension is a larger extension than the closure of an operator.

Application: Using the above Theorem we can show that several operators of interest to us are self-adjoint. Let

- $A_1 = -\Delta$ on $L^2([0,L]^3$ with $D(A_1) = C_c^\infty([0,L]^3)$
- $A_2 = -\Delta$ on $L^2([0,L]^3)$ with $D(A_2) = C_n^\infty([0,L]^3)$

$$= \{ f \in C^\infty([0,L]^3) \mid \underset{\text{normal derivative}}{\nabla_n} f(x) = 0 \text{ for } x \in \partial [0,L]^3 \}$$

- $A_3 = -\Delta + V(x)$ on $L^2([0,L]^3)$ with $D(A_3) = C_c^\infty([0,L]^3)$ or $C_n^\infty([0,L]^3)$

- $A_4 = -\Delta + V(x)$ on $L^2(\mathbb{R}^3)$ with $D(A_4) = \mathcal{C}_c^\infty(\mathbb{R}^3)$

Concerning A_3 and A_4 we will assume that $V \in L^2$ is real-valued and that $d \geq 3$ in case of A_4.

Note that this implies that $V\psi \in L^2$ for $\psi \in \mathcal{C}_c^\infty$. $A_1 - A_4$ are therefore well-defined symmetric operators on their domain. A_1 and A_2 are bounded from below because

$$\langle \phi, -\Delta \phi \rangle = \langle \nabla\phi, \nabla\phi \rangle \geq 0. \qquad (20)$$

The boundary terms vanish by the definition of the domains.

In case of A_3, we have

$$q_3(\phi) = \langle \nabla\phi, \nabla\phi \rangle + \underbrace{\int_{[0,L]^3} V(x) |\phi(x)|^2 \, dx}_{|\ldots| \leq \|V\|_2 \|\phi\|_4^2} . \qquad (21)$$

From the Sobolev inequality (17) we know that $\|\phi\|_6 \leq C \|\phi\|_{H^1}$.

Interpolation: $\|\phi\|_r \leq \|\phi\|_p^\alpha \|\phi\|_q^{1-\alpha}$ if $\frac{1}{r} = \frac{\alpha}{p} + \frac{1-\alpha}{q}$

with $0 \leq \alpha \leq 1$.

$$\frac{1}{4} = \frac{\alpha}{2} + \frac{1-\alpha}{6} \iff \underbrace{\frac{1}{4} - \frac{1}{6}}_{\frac{1}{12}} = \alpha \underbrace{\left(\frac{1}{2} - \frac{1}{6} \right)}_{\frac{1}{3}} \Rightarrow \alpha = \frac{1}{4}$$

That is, $\|\phi\|_4 \leq \|\phi\|_2^{1/4} \|\phi\|_6^{3/4} \leq C \|\phi\|_2^{1/4} \|\phi\|_{H^1}^{3/4}$.

Using $ab \leq \frac{a^p}{p} + \frac{b^q}{q}$ for $a,b \geq 0$, $1<p,q<\infty$ and $\frac{1}{p}+\frac{1}{q}=1$ for the choice $p=4$ and $q=4/3$, we see that

$$\|\phi\|_4^2 \leq C\left(\|\phi\|_2^2 + \|\nabla\phi\|_2^2\right)$$

holds.

$V_2(x) = V(x)\,\mathbb{1}_{\{x \,:\, |V(x)| \leq n(\varepsilon)\}}$

Now write $V = V_1 + V_2$ where $\|V_1\|_2 = \varepsilon$ and $V_2 \in L^\infty$ and estimate

$$q_3(\phi) \geq \langle \nabla\phi, \nabla\phi\rangle - \|V_2\|_\infty \|\phi\|_2^2 - \underbrace{\|V_1\|_2}_{=\varepsilon} C\left(\|\phi\|_2^2 + \|\nabla\phi\|_2^2\right)$$

$$= \langle \nabla\phi, \nabla\phi\rangle\left(1 - C\varepsilon\right) - \|\phi\|_2^2\left(\varepsilon C + \|V_2\|_\infty\right)$$

Choose ε s.t. $C\varepsilon \leq 1/2$

$$\geq \frac{1}{2}\langle \nabla\phi, \nabla\phi\rangle - \text{const.}(\varepsilon)\|\phi\|_2^2. \qquad (22)$$

This shows that $A_3 + \text{const.}(\varepsilon)\|\phi\|_2^2$ is a positive operator.

<u>Exercise</u>: Show that there is a $C>0$ s.t. $q_4(\phi) \geq -C\|\phi\|_2^2$ (23) holds.

Using these bounds (20, 22, 23) and the Theorem of the Friedrichs extension, we see that $A_1 \dots A_4$ have self-adjoint extensions. While the

Theorem does not allow us to get information on the domain of these extensions (other than it is a subset of the form domain), we can obtain their form domains. Let us denote the self-adjoint extensions by $\hat{A}_i$ and their form domains by $\hat{Q}_i$.

Then

- $\hat{Q}_1 = H^1_0([0,L]^d)$ (form domain of Dirichlet Laplacian)
- $\hat{Q}_2 = H^1([0,L]^d)$ (form domain of Neumann Laplacian)
- $\hat{Q}_3 = H^1_0([0,L]^d), H^1([0,L]^d)$ (Exercise)
- $\hat{Q}_4 = H^1(\mathbb{R}^d)$ (Exercise)

In many cases it is sufficient to know the form domain of a self-adjoint extension. A similar consideration is possible if periodic boundary conditions for the Laplacian on $[0,L]^3$ are considered.

4.4. Spectral theorem and variational characterization of eigenvalues

Proposition: Let (M,μ) be a measure space with μ a finite measure. Suppose that f is a measurable real-valued function on M which is finite a.e.. Then the operator $\phi \xrightarrow{T_f} f\phi$ on $L^2(M,\mu)$ with domain

$$D(T_f) = \{\phi \mid f\phi \in L^2(M,\mu)\}$$

is self-adjoint.

<u>Example:</u> $M_x \phi(x) = x\phi(x)$ defined on $L^2(\mathbb{R})$. We have

$$\phi \in D(M_x) \Leftrightarrow \int_{\mathbb{R}} x^2 \, |\phi(x)|^2 dx .$$

The above Proposition identifies a class of self-adjoint operators. The spectral theorem below tells us that we found all of them.

<u>Theorem (Spectral theorem):</u> Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Then there is a measure space $\langle M,\mu\rangle$ with μ a finite measure, a unitary operator $[\langle U\psi, U\varphi\rangle = \langle \psi,\varphi\rangle \ \forall \ \psi,\varphi]$ $U : \mathcal{H} \to L^2(M,\mu)$, and a real-valued function f on M which is finite a.e. so that

(a) $\psi \in D(T) \Leftrightarrow f(\cdot)(U\psi)(\cdot) \in L^2(M,\mu)$,

(b) if $\psi \in U D(T)$, then $(UTU^{-1}\psi)(m) = f(m)\psi(m)$.

Example: Denote by $(\mathcal{U}f)(p) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{ipx} f(x)\,dx$ the Fourier transform on $L^2(\mathbb{R}^d)$. By the Plancherel theorem we have $\langle f, g\rangle = \langle \mathcal{U}f, \mathcal{U}g\rangle$ with the L^2-scalar product. Denote by $-\Delta$ the self-adjoint Laplacian with domain $H^2(\mathbb{R}^d)$. A short computation shows

$$-\Delta = \mathcal{U}^{-1} p^2 \, \mathcal{U} .$$

Theorem: The self-adjoint operators $\hat{A}_1, \hat{A}_2$ and $\hat{A}_3$ that have been introduced on p. 23 have the following properties:

- The measure space $\langle M, \mu\rangle$ in the spectral theorem can in their case be chosen s.t. $M = \mathbb{N}$.
- The function $f: \mathbb{N} \to \mathbb{R}$ can be chosen s.t. $f(1) < f(n)$ for $n > 1$. It has the property that each value is attained only finitely many times and that $f(n) \to \infty$ for $n \to \infty$ holds.

Remark: In other words the operators $\hat{A}_i$ with $i = 1,2,3$ can be written as $\sum_{\alpha=1}^{\infty} \lambda_\alpha P_\alpha$, with eigenvalues $\lambda_1 < \lambda_2 \le \lambda_3 \dots$ and finite dimensional $\underbrace{\text{orthogonal}}_{P^* = P}$ projections $P_1, P_2, \dots$

The projection P_1 has rank 1.

Eigenvalues of a self-adjoint operator $(T, D(T))$ that is bounded from below can be characterized by the following variational principle:

$$\lambda_0 = \inf_{\substack{\psi \in D(T) \\ \|\psi\| = 1}} \langle \psi, T\psi \rangle \qquad \text{minimizer } \psi_0 \text{ is EF of } \lambda_0$$

$$\lambda_1 = \inf_{\substack{\psi \in D(T),\, \psi \perp \psi_0 \\ \|\psi\| = 1}} \langle \psi, T\psi \rangle \qquad \text{minimizer } \psi_1 \text{ is EF of } \lambda_1$$

$$\lambda_3 = \inf_{\substack{\psi \in D(T),\, \psi \perp \{\psi_0, \psi_1\} \\ \|\psi\| = 1}} \langle \psi, T\psi \rangle \qquad \text{minimizer } \psi_2 \text{ is EF of } \lambda_2$$

$$\vdots$$

The above variational principle can be used to compute eigenvalues (e.g. on a computer) and to estimate the first eigenvalue. Estimating other than the lowest eigenvalue is difficult, however, because one needs to know the eigenfunctions of all preceeding eigenvalues, which is rarely the case. The next statement shows a way to obtain this information without knowing the eigenfunctions.

<u>Theorem (min-max principles)</u>: Let $(T, D(T))$ be a self-adjoint operator that can be written as $\sum_{\alpha=1}^{\infty} \lambda_\alpha P_\alpha$ with finite-dimensional projections $\{P_\alpha\}_{\alpha=1}^{\infty}$ and $\inf_{\alpha \geq 1} \lambda_\alpha \geq -C$ for some $C > 0$. The eigenvalues $\{\lambda_\alpha\}_{\alpha=1}^{\infty}$ of T can be characterized by the following two variational principles:

Max-min principle: $$\lambda_n = \max_{\substack{\|\phi_1\|, \dots, \|\phi_{n-1}\| = 1 \\ \phi_1 \dots \phi_{n-1} \in Q(T)}} \; \min_{\substack{\|\phi_n\| = 1 \\ \phi_n \in Q(T)}} \left\{ q(\phi_n) \mid \phi_n \perp \phi_0 \dots \phi_{n-1} \right\}$$

Min-max principle: $$\lambda_n = \min_{\substack{\|\phi_1\|, \dots, \|\phi_{n-1}\| \\ \text{and mutually} \\ \text{orthogonal with} \\ \phi_1 \dots \phi_{n-1} \in Q(T)}} \; \max_{\|\phi\| = 1} \left\{ q(\phi) \mid \phi \in \mathrm{Span}(\phi_1 \dots \phi_{n-1}) \right\}$$

The proof of the above statements is an elementary exercise in linear algebra and can be found in [5], Section 12.1.