Notes on

PDE and Modelling

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Summer Term 2017

These are short incomplete notes. They do not substitute textbooks. The following textbooks are recommended.

- S. Gustafson, I.M. Sigal: Mathematical concepts of quantum mechanics, Springer 2006.
- B. Simon: Operator theory, AMS 2016.
- G. Teschl: Mathematical methods in quantum mechanics, AMS 2014.
- S. Weinberg: Lectures in quantum mechanics, Cambridge 2013.

Additional literatur:

- R. Feynman, Leighton, Sands: The Feynman lectures in physics.
- R. Penrose: The road to reality. Vintage 2005.

Correction are welcome and should be sent to `koch@math.uni-bonn.de` or told me during office hours. The notes are only for participants of the course V3B2/F4B1 *PDE and Modelling* at the University of Bonn, summer term 2017. A current version can be found at
`http://www.math.uni-bonn.de/ag/ana/SoSe17/V3B2_SS_17.html`.

I am very grateful for the support of Xian Liao in preparing these notes.

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Contents

[19.04.2017]

1 Introduction

Around 1900 (Rutherford model, Dynamiden model, Bohr model, Bohr-Sommerfeld model): Positively charged small nucleus contains most of mass, with negatively charged electrons around. There is evidence for a discrete set of energy levels corresponding to sharp spectral lines (stars, heated metal).

Maxwell published around 1861 equations describing basically all electromagnetic effects known at that time:

$$\begin{aligned} \nabla \cdot E &= \frac{1}{\varepsilon_0}\rho \\ \nabla \cdot B &= 0 \\ \nabla \times E &= -\frac{\partial B}{\partial t} \\ \nabla \times B &= \mu_0 j + \mu_0 \varepsilon_0 \frac{\partial E}{\partial t} \end{aligned}$$

where E is the electric field, B is the magnetic field, ρ is the charge density, j is the electric current, $\mu_0\varepsilon_0 = \frac{1}{c^2}$ with permeability μ_0 and permittivity ε_0.

Theory of electromagnetic waves, beautiful theory combining previous complicated special theories of magnetism, elctromagnetic waves and currents.

It immediately implies constant finite speed of light. This was a major motivation for Einstein to develop special and general relativity. However, it leads to a severe conflict with atom models: rotating electrons radiate energy and hence lose energy fast!

Quantum mechanics provides an extremely good description of atoms and molecules. It raises however questions:

1. How does quantum mechanics interact with light? This is answered in quantum electrodynamics.
2. Why is the nucleus stable? Radioactive decay shows that the nucleus consists of smaller parts, which carry a large positive charge on a small area. How can it be stable, when equal charges repel with a force which is the inverse square of the distance? This is answered by quantum gauge theories.

Beyond describing atoms and molecules well quantum mechanics provides insights for the modifications needed for quantum field theories. It is remarkable that a large part of quantum mechanics was developed within around 20 years, with the formulation of quantum mechanics completed around 1925, and quantum theory of light until 1935, with important contributions by Fermi, Heisenberg and Dirac.

1.1 The formalism of quantum mechanics

The formalism was developed by Schrödinger, Heisenberg, Born, Jordan, v. Neumann, Weyl, Dirac: from around 1920 to 1930. Quantum mechanics centers around the Schrödinger equation

$$\begin{aligned} i\hbar\partial_t u + \frac{\hbar^2}{2m}\Delta u &= Vu \qquad \text{on } \mathbb{R}\times\mathbb{R}^d \\ u(0,x) &= u_0(x) \qquad \text{on } \mathbb{R}^d \end{aligned}$$

where $V : \mathbb{R}^d \to \mathbb{R}$ is a potential like $|x|^{-1}$.

If $V = 0$ we obtain a solution in the same way as for the heat equation:

$$u(t,x) = \left(\frac{m}{2\pi i\hbar t}\right)^{\frac{d}{2}} \int_{\mathbb{R}^d} e^{-\frac{im|x-y|^2}{4\hbar t}} u_0(y)dy.$$

Keywords are *Uncertainty relation*, *Wave mechanics*, *Schrödinger equation*. A key step was the *Copenhagen interpretation* of the $|u|^2$ as probability distribution.

Later developments include

- Quantum electrodynamics QED with Dirac as a central figure. It is a relativistic quantum theory.
- Quantum chromodynamics QCD (Gauge theory), quarks and gluons, confinement (no free quark) and asymptotic freedom (Politzer, Wilczek, Gross (Nobel prize 2004)), standard model
- So-called effective quantum field theories deduced from QCD allow to analyse the atomic nucleus, hadrons, protons and neutrons.

Quantum physics leads to an amazing agreement between theory and experiment. Quantum mechanics is a solid mathematical theory, in contrast to quantum electrodynamics. In quantum electrodynamics there is a solid procedure for calculating important quantities. The status of quantum gauge theories looks much less clear to me. It allows to obtain good effective field theories.

However the nature of measurements remains unclear. A quantum theory including gravity seems out of reach at this point. One may wonder whether the situation is comparable to the end of the 19th century, when Maxwell's equations provided an amazing unification and consistent understanding, but with striking puzzles.

1.2 The double slit experiment: Wave particle duality

At the end of the 19th century Planck described black-body radiation. Black body radiation and the photoelectric effect remained mysterious when electromagnetic waves were considered as waves. The photoelectric effect led Einstein to the hypothesis that light has a particle character in certain situations (Nobel Prize in 1921). The particles are called photons in 1926 by Wolfers and Lewis. Compton performed experiments which showed that photons scatter at electronics, leading to the Nobel prize in 1927. Currently Meschede (Bonn) is working with quantum systems of around 100 photons at temperatures 10^{-6} degree Kelvin.

On the other hand Louis de Broglie, Bohr and others realised that particles behave like waves. The most intriguing thought experiment is the double slit experiment. If we fix the frequency (colour) of the light, and reduce the intensity, then a light source emits single photons.

Let us send the photons through a double slit. Waves sent through a slit showed an intricate pattern on a screen. With a double slit there is some interference from both slits.

It turns out that the interference pattern does not change even if we make sure that the single photons hit the screen one by one. The patter is not the sum of two single slits! So mysteriously light behaves wavelike even if we know that there is only one photon at a time!

This thought experiment has been realized with electrons by Thomson and Davisson, Germer in 1927 (Nobel Prize for Davisson and Thomson in 1937). A spectacular point was Zeilinger et al (1999, Nature: Wave-particle duality of C_{60}(Fullerene)).

1.3 Outline

2. The Fourier transform

3. Selfadjoint operators

4. Examples: Free particles, the harmonic oscillator and the hydrogen atom.

5. Symmetry groups
6. Scattering
7. Multiparticle systems

2 The Fourier transform

2.1 The definition in L^1

Recall: Fourier series in one dimension. Let $f \in L^2_{loc}(\mathbb{R})$ be 2π periodic. It can be formally written as

$$f = \sum_{k\in\mathbb{Z}} a_k e^{ikx}$$

with

$$a_k = \frac{1}{2\pi}\int_{\mathbb{R}} f(x)e^{-ikx}dx.$$

By Plancherel's formula

$$\|f\|^2_{L^2(0,2\pi)} = 2\pi \sum_{k\in\mathbb{Z}} |a_k|^2.$$

Fourier series express a periodic function in terms of pure harmonics e^{ikx} with frequency k.

Definition 2.1. *Let $f \in L^1(\mathbb{R}^d;\mathbb{C})$. We define its Fourier transform by*

$$\hat{f}(k) = \mathcal{F}(f)(k) = (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} f(x)e^{-ik\cdot x}dx$$

for $k \in \mathbb{R}^d$.

Lemma 2.2 (Riemann-Lebesgue)**.** *Let $f \in L^1(\mathbb{R}^d;\mathbb{C})$. The Fourier transform $\hat{f}$ is continuous and satisfies*

$$\lim_{|k|\to\infty} \hat{f}(k) = 0.$$

Proof. Let $f \in L^1(\mathbb{R}^d;\mathbb{C})$ and $k_j \to k$. Then

$$f(x)e^{-ik_j\cdot x} \to f(x)e^{-ik\cdot x}$$

for every $x \in \mathbb{R}^d$ and

$$|f(x)e^{-ik\cdot x}| = |f(x)|,$$

hence $|f|$ is an integrable majorant. By the convergence theorem of Lebesgue

$$\int_{\mathbb{R}^d} f(x)e^{-ik_j\cdot x}dx \to \int_{\mathbb{R}^d} f(x)e^{-ik\cdot x}dx$$

and hence $k \to \hat{f}(k)$ is continuous.

Since $f \in L^1(\mathbb{R}^d;\mathbb{C})$ there exists a sequence $f_j \in C_0^\infty(\mathbb{R}^d;\mathbb{C})$ of smooth functions with compact support with $f_j \to f$ in $L^1(\mathbb{R}^d;\mathbb{C})$. Then

$$\left|\int_{\mathbb{R}^d} f_j(x)e^{-ik\cdot x}dx - \int_{\mathbb{R}^d} f(x)e^{-ik\cdot x}dx\right| \leqslant \int_{\mathbb{R}^d} |f_j(x) - f(x)|dx \to 0$$

uniformly in k. Hence it suffices to prove that

$$\int_{\mathbb{R}^d} f_j(x)e^{-ik\cdot x}dx \to 0 \qquad \text{as } |k| \to \infty.$$

If the lth component $k_l \neq 0$ then for any $f \in C_0^\infty(\mathbb{R}^d;\mathbb{C})$,

$$\int_{\mathbb{R}^d} f(x)e^{-ik\cdot x}dx = \int_{\mathbb{R}^d} f(x)\frac{1}{-ik_l}\partial_{x_l}e^{-ik\cdot x}dx = \frac{1}{ik_l}\int_{\mathbb{R}^d}(\partial_{x_l}f)e^{-ik\cdot x}dx$$

which tends to 0 as $|k_l|$ tends to ∞. □

The Fourier transform is a continuous linear map from $L^1(\mathbb{R}^d)$ to $C_0(\mathbb{R}^d)$, the space of continuous functions decaying at ∞. Trivially, with $C_b(\mathbb{R}^d)$ the space of bounded continuous functions equipped with the supremums norm

$$\|\hat{f}\|_{C_b(\mathbb{R}^d)} \leqslant (2\pi)^{-\frac{d}{2}}\|f\|_{L^1(\mathbb{R}^d)}.$$

We recall the definition of the convolution

$$f * g(x) = \int_{\mathbb{R}^d} f(x-y)g(y)dy$$

which satisfies (assuming that the convolution is a measurable function),

$$\begin{aligned}
\|f * g\|_{L^1} &= \int_{\mathbb{R}^d}\left|\int_{\mathbb{R}^d} f(x-y)g(y)dy\right|dx \\
&\leqslant \int_{\mathbb{R}^{2d}} |f(x-y)||g(y)|dydx \\
&= \int_{\mathbb{R}^d} |g(y)|\int_{\mathbb{R}^d}|f(x-y)|dxdy \\
&= \|f\|_{L^1}\|g\|_{L^1}
\end{aligned}$$

by a multiple application of the theorem of Fubini. More generally Young's inequality

$$\|f * g\|_{L^r(\mathbb{R}^d)} \leqslant \|f\|_{L^p(\mathbb{R}^d)}\|g\|_{L^q(\mathbb{R}^d)}$$

holds whenever $1 \leqslant p, q, r \leqslant \infty$ and

$$\frac{1}{p} + \frac{1}{q} = 1 + \frac{1}{r}.$$

The convolution is commutative $f * g = g * f$ and associative $(f * g) * h = f*(g*h)$ and can be defined for distributions (see Lecture notes on Functional Analysis and PDE, or Lieb and Loss: Analysis).

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We also have

$$\mathcal{F}(f * g)(k) = (2\pi)^{\frac{d}{2}}(\hat{f}\hat{g})(k) \tag{2.1}$$

for $f, g \in L^1(\mathbb{R}^d)$. This is seen by the calculation

$$\begin{aligned}
&(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-ik\cdot x} \int_{\mathbb{R}^d} f(x-y)g(y)dydx \\
&= (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-ik\cdot y} g(y) \int_{\mathbb{R}^d} e^{-ik\cdot(x-y)} f(x-y)dx\,dy \\
&= (2\pi)^{\frac{d}{2}} \hat{g}(k)\hat{f}(k).
\end{aligned}$$

Let A^t be the transpose of a matrix and A^{-t} the inverse of the transpose (if it is invertible).

Lemma 2.3. *Let A be a real invertible $d \times d$ matrix and $f \in L^1(\mathbb{R}^d)$. Then*

$$\mathcal{F}(f \circ A)(k) = |\det A|^{-1}\hat{f}(A^{-t}k).$$

Moreover

$$\mathcal{F}(f(.+h))(k) = e^{ik\cdot h}\hat{f}(k), \quad \forall h \in \mathbb{R}^d.$$

Proof. Exercise. □

The Fourier transform of finite Borel measures μ is defined by

$$(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-ik\cdot x} d\mu(x).$$

A particular case is the Dirac measure with

$$\hat{\delta}_0 = (2\pi)^{-\frac{d}{2}}.$$

It acts as identity under the convolution.

2.2 The Schwartz space

In this subsection we study the Fourier transform of smooth decaying functions. This simplifies formal manipulations.

Definition 2.4 (Schwartz functions)**.** *A function $f \in C^\infty(\mathbb{R}^d;\mathbb{C})$ is a Schwartz function if for every multiindices α and β the function*

$$x^\alpha \partial^\beta f$$

is bounded. The space of Schwartz functions is denoted by $\mathcal{S}(\mathbb{R}^d)$. We say f_n converges to f in $\mathcal{S}(\mathbb{R}^d)$ if for every multiindices α and β

$$x^\alpha \partial^\beta f_n \to x^\alpha \partial^\beta f$$

uniformly in x.

First properties are:

1. $f \in \mathcal{S}(\mathbb{R}^d)$ implies $x_j f \in \mathcal{S}(\mathbb{R}^d)$ and $\partial_{x_j} f \in \mathcal{S}(\mathbb{R}^d)$.
2. $f \in \mathcal{S}(\mathbb{R}^d)$ and $g \in C_b^\infty(\mathbb{R}^d)$ implies $gf \in \mathcal{S}(\mathbb{R}^d)$.
3. $f \in \mathcal{S}(\mathbb{R}^d)$ and $g \in L^1$ with compact support implies $f * g \in \mathcal{S}(\mathbb{R}^d)$.
4. $f \in \mathcal{S}(\mathbb{R}^d)$ and g a distribution with compact support implies $f * g \in \mathcal{S}(\mathbb{R}^d)$: Suppose g is supported on $K \subset \mathbb{R}^d$ compact. Then there exist C and k so that
$$|g(\phi)| \leqslant C \sup_{|\alpha| \leqslant k, x \in K} |\partial^\alpha \phi(x)|.$$
Since
$$f * g(x) = \int_{\mathbb{R}^d} f(x-y) g(y) dy = g(f(x - .))$$
we obtain that
$$|x^\gamma \partial^\beta (f * g)(x)| \leqslant C \sup_{x, |\alpha| \leqslant k} \sup_{z \in K} |(x+z)^\gamma \partial^{\alpha+\beta} f(x)|$$
is uniformly bounded.
5. $f \in \mathcal{S}(\mathbb{R}^d)$ implies $f \in L^p(\mathbb{R}^d)$ for $1 \leqslant p \leqslant \infty$. Moreover $f_j \to f$ in $\mathcal{S}(\mathbb{R}^d)$ implies $f_j \to f$ in L^p for all $1 \leqslant p \leqslant \infty$.
6. $f, g \in \mathcal{S}$ imples $f * g \in \mathcal{S}$.
7. Gaussian functions $e^{-\frac{1}{2}|x|^2}$ are Schwartz functions.

Lemma 2.5. *Let $f \in \mathcal{S}(\mathbb{R}^d)$. Then $\hat{f} \in \mathcal{S}(\mathbb{R}^d)$ and*

$$\mathcal{F}(x_j f)(k) = i\partial_{k_j} \hat{f}(k) \tag{2.2}$$

$$\mathcal{F}(\partial_j f)(k) = ik_j \hat{f}(k) \tag{2.3}$$

If also $g \in L^1$ then

$$\mathcal{F}(f * g)(k) = (2\pi)^{\frac{d}{2}} \hat{f}(k)\hat{g}(k) \tag{2.4}$$

and

$$\mathcal{F}(fg)(k) = (2\pi)^{-\frac{d}{2}} \hat{f}(k) * \hat{g}(k) \tag{2.5}$$

Proof. We first prove the first two formulas:

$$(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} x_j f(x) e^{-ik\cdot x} dx = (2\pi)^{-\frac{d}{2}} i \int_{\mathbb{R}^d} f(x) \partial_{k_j} e^{-ik\cdot x} dx = i\partial_{k_j} \hat{f}(k)$$

and by integration by parts, and by application of the theorem of Fubini

$$(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} \partial_{x_j} f(x) e^{-ik\cdot x} dx = (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} -f(x) \partial_{x_j} e^{-ik\cdot x} dx = ik_j \hat{f}(k).$$

We recall that $f \in \mathcal{S}(\mathbb{R}^d)$ and we want to verify that $\hat{f} \in \mathcal{S}(\mathbb{R}^d)$. Let α and β be multiindices. Then, by a recursive application of the previous formulas

$$k^\alpha \partial_k^\beta \hat{f}(k) = (-i)^{|\alpha|+|\beta|} \mathcal{F}(\partial_x^\alpha x^\beta f)(k)$$

which is the Fourier transform of a Schwartz functions, and hence bounded. Thus $\hat{f} \in \mathcal{S}(\mathbb{R}^d)$. We have already proven the third formula for L^1 functions, which implies the third formula here. The last formula will be a consequence of the inversion formula. □

We want to calculate several Fourier transforms. We recall that (see also the appendix)

$$\int_{\mathbb{R}^d} e^{-\frac{1}{2}|x|^2} dx = (2\pi)^{\frac{d}{2}}.$$

On the other side, $\mathcal{F}(e^{-\frac{1}{2}|x|^2})$ satisfies the following equation

$$0 = \mathcal{F}(\partial_{x_j} e^{-\frac{1}{2}|x|^2} + x_j e^{-\frac{1}{2}|x|^2}) = i(\partial_{k_j} + k_j)\mathcal{F}(e^{-\frac{1}{2}|x|^2})(k).$$

The differential equation

$$\partial_t \phi + t\phi = 0$$

is linear, of first order, and it has a one dimensional space of solutions: There exists C so that

$$\phi = Ce^{-\frac{1}{2}t^2}.$$

Hence we obtain recursively

$$\mathcal{F}(e^{-\frac{1}{2}|x|^2}) = \phi_{d-1}(x_1, \dots x_{d-1})e^{-\frac{1}{2}|x_d|^2} = ce^{-\frac{1}{2}\sum_{j=1}^{d} x_j^2}.$$

Since

$$\mathcal{F}(e^{-\frac{1}{2}|x|^2})(0) = (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-\frac{1}{2}|x|^2} dx = 1$$

we obtain

$$\mathcal{F}(e^{-\frac{1}{2}|x|^2}) = e^{-\frac{1}{2}|k|^2}. \tag{2.6}$$

Now let $d = 1$ and

$$f = \begin{cases} e^{-x} & \text{if } x > 0 \\ 0 & \text{if } x \leqslant 0. \end{cases}$$

Then

$$\hat{f}(k) = (2\pi)^{-\frac{1}{2}} \frac{1}{1+ik}.$$

Now let $f(x) = e^{-|x|}$. The same calculation shows that

$$\hat{f}(k) = (2\pi)^{-\frac{1}{2}} (\frac{1}{1+ik} + \frac{1}{1-ik}) = \sqrt{2/\pi} \frac{1}{1+k^2}.$$

Now let $f(x) = (1+|x|^2)^{-1}$. It is integrable. Let $k < 0$. Then

$$\begin{aligned} \int_{-\infty}^{\infty} e^{-ikx}(1+x^2)^{-1} dx &= \lim_{R\to\infty} \int_{-R}^{R} e^{-ikx}(1+x^2)^{-1} dx \\ &= \lim_{R\to\infty} \int_{\gamma} e^{-ikz}(1+z^2)^{-1} dz \end{aligned}$$

where γ is the clockwise path around the upper semidisk of radius R (this is true since $k < 0$). Now

$$(z^2+1)^{-1} = \frac{1}{2i}(\frac{1}{z-i} - \frac{1}{z+i}).$$

Let $U \subset \mathbb{C}$ and $f : U \to \mathbb{C}$. It is holomorphic if it is everywhere differentiable and satisfies the Cauchy-Riemann differential equations,

$$\partial_x \operatorname{Re} f = \partial_y \operatorname{Im} f, \partial_y \operatorname{Re} f = -\partial_x \operatorname{Im} f.$$

Let $U \subset \mathbb{C}$ have a smooth boundary. Let γ_0 be the path defined by the boundary with the orientation so that U is always on the left. The Cauchy integral theorem says that if f is holomorphic on V, $\overline{U} \subset V$ and U is simply connected then

$$\int_{\gamma_0} f dz = 0.$$

By the Cauchy integral theorem

$$\int_\gamma e^{-ikz} \frac{1}{z+i} dz = 0.$$

By the residue theorem (or as a consequence of the Cauchy integral theorem)

$$\int_\gamma e^{-ikz} \frac{1}{z-i} dz = 2\pi i e^k.$$

We obtain (with a similar argument for $k > 0$)

$$\hat{f}(k) = \sqrt{\pi/2} e^{-|k|}.$$

[21.04.2017]

[26.04.2017]

2.3 Fourier inversion

We begin with two simple calculations.

Lemma 2.6. *Let $f, g \in L^1(\mathbb{R}^d)$. Then*

$$\int_{\mathbb{R}^d} f \hat{g} dx = \int_{\mathbb{R}^d} \hat{f} g dk, \tag{2.7}$$

and, for $m \in \mathbb{R}^d$,

$$\widehat{e^{im\cdot x} f} = \hat{f}(k - m).$$

We have for $a > 0$

$$\mathcal{F}(e^{-\frac{a^2}{2}|x|^2}) = a^{-d} e^{-\frac{1}{2a^2}|k|^2}.$$

Proof. Both sides of the first equality are equal to

$$(2\pi)^{-d/2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(x) g(k) e^{-ik\cdot x} dk dx.$$

The second equality is a direct calculation:

$$(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{im\cdot x} f(x) e^{-ik\cdot x} dx = (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-i(k-m)\cdot x} f(x) dx.$$

The third equality is a special cases of exercises. $\square$

Definition 2.7. *Let $f \in L^1(\mathbb{R}^d)$. We define*

$$\check{f}(x) = \mathcal{F}^{-1}(f)(x) = (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} f(k)e^{ik\cdot x}dk.$$

We will see that this map is the inverse of the Fourier transform, which will justify the notation. Clearly $\check{f}(k) = \hat{f}(-k)$. All the previous results have analogues for $\mathcal{F}^{-1}$.

Theorem 2.8. *Let $f \in \mathcal{S}(\mathbb{R}^d)$, Then*

$$\mathcal{F}^{-1}\mathcal{F}(f)(x) = f(x) = \mathcal{F}\mathcal{F}^{-1}(f)(x).$$

Proof. Let $f \in \mathcal{S}(\mathbb{R}^d)$. We calculate

$$\begin{aligned}(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} \hat{f}(k)e^{ik\cdot x}dk &= \lim_{\varepsilon\to 0}(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-\frac{\varepsilon^2}{2}|k|^2+ik\cdot x}\hat{f}(k)dk \\ &= \lim_{\varepsilon\to 0}\int_{\mathbb{R}^d} (2\pi)^{-\frac{d}{2}}\varepsilon^{-d}e^{-\frac{1}{2\varepsilon^2}|x-y|^2}f(y)dy \\ &= f(x).\end{aligned}$$

We explain the above calculation one equality by one: The first equality follows by pointwise convergence; For the second one we apply the first statement of Lemma 2.6 with $g_\varepsilon = e^{-\frac{\varepsilon^2}{2}|k|^2+ik\cdot x}$, where by the second and third statement of Lemma 2.6

$$\hat{g}_\varepsilon(y) = \varepsilon^{-d}e^{-\frac{1}{2\varepsilon^2}|y-x|^2};$$

The last equality holds since $\hat{g}_\varepsilon$ is a Dirac sequence. □

In particular the inverse of the Fourier transform represents a function as sum resp. integral of complex exponentials. Again the symmetry between functions and their Fourier transform is visible. The formula (2.5)

$$\widehat{fg} = (2\pi)^{-\frac{d}{2}}\hat{f} * \hat{g}$$

is equivalent to (2.4)

$$\widehat{f * g} = (2\pi)^{\frac{d}{2}}fg.$$

Equation (2.7) has more interesting consequences.

Theorem 2.9. *Let $f, g \in \mathcal{S}(\mathbb{R}^d)$. Then*

$$\int_{\mathbb{R}^d} f\bar{g}dx = \int_{\mathbb{R}^d} \hat{f}\overline{\hat{g}}dk,$$

and the Fourier transform defines a unitary operator from $L^2(\mathbb{R}^d)$ to itself.

Proof. This follows from

$$\int_{\mathbb{R}^d} f\bar{\hat{\hat{g}}}dx = \int_{\mathbb{R}^d} f\hat{\bar{\hat{g}}}dx = \int_{\mathbb{R}^d} \hat{f}\bar{\hat{g}}dk.$$

In particular

$$\|f\|_{L^2} = \|\hat{f}\|_{L^2}.$$

Let $f \in L^2$. There exists a sequence $f_n \in \mathcal{S}$ with $f_n \to f$ in L^2. Then $\hat{f}_n$ is a Cauchy sequence and there is a unique limit in L^2. We define the Fourier transform of f as this limit. This is a unitary operator. □

It is not hard to check that

$$\mathcal{F}(\mathcal{F}(f))(x) = f(-x)$$

and hence the fourth power of the Fourier transform is the identity.

Lemma 2.10. *We can decompose any function f in $L^2(\mathbb{R}^d;\mathbb{C})$ into*

$$f = f_1 + f_{-1} + f_i + f_{-i}$$

so that

$$\|f\|_{L^2}^2 = \|f_1\|_{L^2}^2 + \|f_{-1}\|_{L^2}^2 + \|f_i\|_{L^2}^2 + \|f_{-i}\|_{L^2}^2$$

and

$$\hat{f}_1 = f_1, \quad \hat{f}_{-1} = -f_{-1}, \quad \hat{f}_i = if_i, \qquad \hat{f}_{-i} = -if_{-i}.$$

The decomposition is unique.

The proof is an exercise.

We have seen that $\mathcal{F}e^{-\frac{|x|^2}{2}} = e^{-\frac{|k|^2}{2}}$. Since

$$f := x_j e^{-\frac{|x|^2}{2}} = \frac{1}{2}(x_j - \partial_{x_j})e^{-\frac{|x|^2}{2}}$$

we have

$$\hat{f} = \frac{i}{2}(\partial_{k_j} - k_j)e^{-\frac{|k|^2}{2}} = -if(k)$$

and similarly, for multiindices α

$$h_\alpha(x) = [\frac{1}{2}(x-\partial)]^\alpha e^{-\frac{|x|^2}{2}} = H_\alpha(x)e^{-\frac{|x|^2}{2}}$$

we have

$$H_\alpha = h_\alpha e^{\frac{|x|^2}{2}} \text{ and } \widehat{h_\alpha} = (-i)^{|\alpha|}h_\alpha.$$

The functions h_α are called Hermite functions and H_α are the Hermite polynomials.

[26.04.2017]

[28.04.2017]

2.4 Tempered distributions

Lemma 2.11. *The Fourier transform defines a continuous map from $\mathcal{S}$ to $\mathcal{S}$.*

Proof. This is an immediate consequence of the continuity $\mathcal{F} : L^1 \to C_b$ and the formula

$$k^\alpha \partial_k^\beta \hat{f}_n = i^{|\alpha|+|\beta|} \widehat{\partial_x^\alpha x^\beta f_n}.$$

$\square$

Lemma 2.12. *Let $f \in \mathcal{S}(\mathbb{R}^d)$. Then*

$$e^{-\frac{1}{2n^2}|x|^2} f \to f \qquad \text{in } \mathcal{S}(\mathbb{R}^d) \text{ as } n \to \infty$$

and

$$(2\pi)^{-\frac{d}{2}} n^d e^{-\frac{n^2}{2}|x|^2} * f \to f \qquad \text{in } \mathcal{S}(\mathbb{R}^d) \text{ as } n \to \infty.$$

Proof. The statements exchange their roles under the Fourier transform. It suffices to prove the first claim. Since

$$|\partial^\alpha e^{-\frac{1}{2n^2}|x|^2}| \leqslant \Big(\sup_y |\partial^\alpha e^{-\frac{1}{2}|y|^2}|\Big) |n|^{-|\alpha|},$$

then

$$|x^\alpha \partial^\beta (e^{-\frac{1}{2n^2}|x|^2} f - f)| = \left| \sum_{\beta_1+\beta_2} c_{\beta_1,\beta} \Big[\partial^{\beta_1}(e^{-\frac{1}{2n^2}|x|^2} - 1)\big(x^\alpha \partial^{\beta_2} f\big)\Big] \right| \leqslant c_{\beta,f} n^{-1}$$

uniformly in x. This is clear if $\beta_1 > 0$. If $\beta_1 = 0$ we use

$$|e^{-\frac{1}{2n^2}|x|^2} - 1| \leqslant \frac{|x|^2}{2n^2}.$$

$\square$

Definition 2.13. *A tempered distribution is a continuous linear map from $\mathcal{S}(\mathbb{R}^d)$ to $\mathbb{C}$. We denote the set of tempered distributions by $\mathcal{S}^*(\mathbb{R}^d)$. We say that $T_j \to T \in \mathcal{S}^*(\mathbb{R}^d)$ if*

$$T_j(f) \to T(f)$$

for all $f \in \mathcal{S}(\mathbb{R}^d)$.

Remarks.

1. We call T continuous if $f_j \to f$ in $\mathcal{S}$ then $T(f_j) \to T(f)$.

2. It is a consequence of the uniform boundedness principle that for $T \in \mathcal{S}^*(\mathbb{R}^d)$ there exist C and N so that

$$|Tf| \leqslant C \sup_{|\alpha|+|\beta|\leqslant N} \sup_x |x^\alpha \partial^\beta f(x)| \tag{2.8}$$

and if $T_j \to T$ there exists N so that

$$\lim_{j\to\infty} \sup\{|Tf - T_j f| : \sup_{|\alpha|+|\beta|\leqslant N} \sup_x |x^\alpha \partial^\beta f(x)| \leqslant 1\} = 0.$$

3. Every function $f \in L^1(\mathbb{R}^d)$ defines a tempered distribution $T_f \in \mathcal{S}^*(\mathbb{R}^d)$ by $T_f(g) = \int_{\mathbb{R}^d} fg dx$.

Definition 2.14. *Let $\phi \in C_b^\infty$ be a smooth function with bounded derivatives and $T \in \mathcal{S}^*$. We define the product by*

$$\phi T(f) = T(\phi f),$$

the derivative by

$$(\partial_{x_j} T)(f) = -T(\partial_{x_j} f),$$

and the convolution with a Schwartz function f by

$$T * f(x) = T(f(x - .)).$$

We define the Fourier transform by

$$\hat{T}(f) = T(\hat{f}), \quad \check{T}(f) = T(\check{f}), \quad f \in \mathcal{S}.$$

Lemma 2.15. *Whenever the operations are allowed we have*

$$\begin{aligned} \partial_{x_j} T_f &= T_{\partial_{x_j} f} \\ \phi T_f &= T_{\phi f} \\ T_g * f &= f * g \\ \hat{T}_f &= T_{\hat{f}} \\ \check{\hat{T}} = \hat{\check{T}} &= T. \end{aligned}$$

All (reasonable) maps are continuous. Moreover, given T there exists N so that

$$|\partial^\alpha T * f(x)| \leqslant c_f (1 + |x|^2)^N, \quad \forall \alpha, \quad \forall f \in \mathcal{S}.$$

Proof. We only prove some typical statements:

$$\partial_{x_j} T_f(\phi) = -T_f(\partial_{x_j}\phi) = -\int_{\mathbb{R}^d} f\partial_{x_j}\phi dx = \int_{\mathbb{R}^d} \partial_{x_j} f\phi dx = T_{\partial_{x_j} f}(\phi),$$

$$\check{\hat{T}}(\phi) = \hat{T}(\check{\phi}) = T(\hat{\check{\phi}}) = T(\phi).$$

Since

$$\partial^\alpha T * f = T * (\partial^\alpha f),$$

it suffices to consider $\alpha = 0$ for the second statement:

$$\begin{aligned}|T * f(x)| = |T(f(x - \cdot))| &\leqslant C \sup_{|\gamma|+|\beta|\leqslant N} \sup_y |(x-y)^\gamma \partial^\beta f(y)| \\ &\leqslant c \sup_{|\gamma|\leqslant N} \sup_y \frac{|x-y|^{|\gamma|}}{(1+|y|^2)^N} \Big(\sup_{|\beta|\leqslant N} \sup_y (1+|y|^2)^N |\partial^\beta f(y)| \Big) \\ &\leqslant c_f (1+|x|^2)^N\end{aligned}$$

where we used that the polynomial $(1+|y|^2)^N$ is a sum of monomials, in the same way as every polynomial. □

Lemma 2.16. *$\mathcal{S}(\mathbb{R}^d)$ is dense in $\mathcal{S}^*(\mathbb{R}^d)$.*

Proof. For all $f \in \mathcal{S}(\mathbb{R}^d)$

$$(2\pi)^{-\frac{d}{2}} n^d e^{-\frac{n^2}{2}|x|^2} * (e^{-|x|^2/m^2} f) \to f \qquad \text{in } \mathcal{S}$$

as $m \to \infty$ and $n \to \infty$. Thus

$$e^{-|x|^2/m^2} \big[(2\pi)^{-\frac{d}{2}} n^d e^{-\frac{n^2}{2}|x|^2} * T\big] \to T$$

in $\mathcal{S}^*$. The convolution in the bracket satisfies a polynomial bound, and hence the left hand side is in $\mathcal{S}$. □

Definition 2.17. *Let T be a (tempered) distribution. The support of T is the complement of all points x for which there exists $r > 0$ so that*

$$Tf = 0$$

whenever $\operatorname{supp} f \in B_r(x)$.

As consequence we have $fT = 0$ and $T(f) = 0$ whenever $\operatorname{supp} f \cap \operatorname{supp} T = \{\}$ (this can be seen by a partition of unity).

Lemma 2.18. *The tempered distribution T is supported in $x = 0$ if and only if $\hat{T}$ is a polynomial.*

Proof. By Lemma 2.8 there exists N so that

$$|Tf| \leqslant c \sup_{|\alpha|+|\beta|\leqslant N} \sup_x |x^\beta \partial^\alpha f(x)|.$$

We fix a function η supported on $B_1(0)$, identically 1 in $B_{\frac{1}{2}}(0)$. Then

$$Tf = T(\eta f) + T(f - \eta f)$$

where the second term vanishes since the intersection of the supports is empty. Thus

$$|Tf| \leqslant c \sup_{|\alpha|\leqslant N} \sup_{|x|\leqslant 1} |\partial^\alpha f(x)|.$$

Now suppose that $\partial^\alpha f(0) = 0$ for $|\alpha| \leqslant N$ and we show $Tf = 0$. Indeed, for any $|\alpha| \leqslant N$ and any $\varepsilon > 0$, using that the product is supported in $B_\varepsilon(0)$ and Taylor's formula for f

$$\begin{aligned} |\partial^\alpha \eta(x/\varepsilon) f| &= |\sum_{\beta+\gamma=\alpha} c_{\beta,\gamma} \partial^\beta \eta(x/\varepsilon) \partial^\gamma f(x)| \\ &\leqslant c_\eta \sum_{\beta+\gamma=\alpha} \varepsilon^{-|\beta|} \sup_{|x|\leqslant\varepsilon} C|x|^{N+1-|\gamma|} \leqslant c\varepsilon^{N+1-|\alpha|}, \end{aligned}$$

we obtain by letting $\varepsilon \to 0$

$$Tf = 0.$$

Now let

$$a_\alpha = \frac{1}{\alpha!} T(\eta x^\alpha).$$

Then, for $f \in \mathcal{S}$

$$Tf = T\left(f - \sum_{|\alpha|\leqslant N} \frac{\partial^\alpha f}{\alpha!}(0) x^\alpha \right) + \sum_{|\alpha|\leqslant N} a_\alpha \partial^\alpha f(0).$$

The first term vanishes by the previous argument and we arrive at

$$Tf = \sum_{|\alpha|\leqslant N} a_\alpha \partial^\alpha f(0) = \sum_{|\alpha|\leqslant N} a_\alpha (-1)^{|\alpha|} (\partial^\alpha \delta_0)(f)$$

and

$$\hat{T}(k) = (2\pi)^{-d/2} \sum_{|\alpha|\leqslant N} a_\alpha (-1)^{|\alpha|} (-ik)^\alpha.$$

The opposite direction is immediate. $\square$

2.5 Periodic distributions

Definition 2.19. *Let $Z \subset \mathbb{R}^d$ be a lattice (i.e. a discrete group whose span is $\mathbb{R}^d$). A (tempered) distribution T is called Z periodic, if*

$$T(\phi) = T(\phi(.+h))$$

for every $h \in Z$.

We define the dual lattice

$$Z^* = \{k \in \mathbb{R}^d : k \cdot h \in 2\pi\mathbb{Z} \quad \text{for all } h \in Z\}.$$

Lemma 2.20. *T is Z periodic if and only if $\hat{T}$ is a sum of Dirac measures in Z^*.*

Proof. Suppose that T is Z periodic. Then

$$T(\phi) = T(\phi(.+h))$$

hence

$$\hat{T}(\phi) = T(\hat{\phi}) = T(\hat{\phi}(.+h)) = \hat{T}(e^{-ih\cdot}\phi)$$

and

$$\hat{T}((1-e^{-ih\cdot})\phi) = 0$$

for all $h \in \mathbb{Z}$. Let $h_j \in Z$ be a basis. If $x_0 \notin Z^*$ we can define h_j so that $h_j \cdot x_0 \neq 0$, i.e. $h_j \cdot x_0 \notin 2\pi\mathbb{Z}$. Let ϕ be supported in a small neighborhood of x_0 so that $\phi/(1-e^{ih_j\cdot x})$ is smooth and bounded. Then

$$\hat{T}\phi = \hat{T}\big((1-e^{ih_j\cdot x})\,(\phi/(1-e^{ix\cdot h_j}))\big) = 0.$$

Thus $\hat{T}$ is supported in Z^*.

A linear change of coordinates maps Z to $2\pi\mathbb{Z}^d$ and Z^* to $\mathbb{Z}^d$. It suffices to consider this situation. It also suffices to prove that $\eta\hat{T}$ is a Dirac measure for $\eta \in C_0^\infty$ supported in a ball of radius $1/2$ around 0. We pick η with $\eta(0) = 1$. Suppose $f \in \mathcal{S}$ vanishes at $x = 0$. By the fundamental theorem of calculus

$$f(x) = f(0) + \int_0^1 x \cdot Df(tx)dt$$

and hence

$$\eta f(x) = \eta \sum_{j=1}^d (1-e^{ix_j}) \frac{x_j}{1-e^{ix_j}} \int_0^1 \partial_j f(tx)dt$$

and

$$\eta\hat{T}(f) = \sum_{j=1}^{d} \hat{T}((1-e^{ix_j})f_j) = 0$$

where we combined the obvious terms into f_j. For general f we obtain

$$\eta\hat{T}(f) = \eta\hat{T}(f - f(0)\eta) + f(0)\eta\hat{T}(\eta) = \hat{T}(\eta^2)\delta_0(f).$$

□

A special case is $T = \sum_{k\in\mathbb{Z}^d} \delta_{2\pi k}$. It is periodic and a sum of Dirac measures. Thus exists c such that

$$\hat{T} = c\sum_{k\in\mathbb{Z}^d} \delta_k.$$

Lemma 2.21 (Poisson summation formula)**.** *Let $f \in \mathcal{S}$. Then*

$$\sum_{y\in 2\pi\mathbb{Z}^d} f(y) = \sum_{k\in\mathbb{Z}^d} \hat{f}(k). \tag{2.9}$$

Proof. Let

$$F(x) = \sum_{y\in 2\pi\mathbb{Z}^d} f(x+y).$$

It is 2π periodic and hence

$$F(x) = \sum_{k\in\mathbb{Z}^d} a_k e^{ikx}$$

with

$$a_k = (2\pi)^{-\frac{d}{2}} \int_{(0,2\pi)^d} F(x)e^{-ik\cdot x}dx = (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} f(x)e^{-ik\cdot x}dx = \hat{f}(k).$$

Thus

$$\sum_{y\in 2\pi\mathbb{Z}^d} f(y) = F(0) = \sum_{k\in\mathbb{Z}^d} a_k = \sum_{k\in\mathbb{Z}^d} \hat{f}(k).$$

□

[28.04.2017]

[03.05.2017]

3 Selfadjoint operators and unitary groups

The formulation of quantum mechanics uses unbounded selfadjoint operators on a Hilbert space H. We want to describe systems with a number of symmetries: Translation symmetry and rotation symmetry for free particles, inner symmetries for example between proton and neutron for the strong force, or spin, the symmetry between identical particles. It is a basic principle of quantum mechanics that symmetries act by unitary operators on the Hilbert space.

The simplest example is the translation group

$$h \to U(h) \text{ where } h \in \mathbb{R}^d, \quad U(h) : H \mapsto H,$$

with the properties

$$U(h_1 + h_2) = U(h_1)U(h_2)$$
$$U(0) = 1_H$$
$$(U(h))^* = U(-h).$$

For every $\phi \in H$ the map

$$h \to U(h)\phi$$

is continuous. Suppose that $d = 1$ and $h \in \mathbb{R}$. Stone's theorem gives a one to one correspondence between one parameter unitary groups and unbounded self adjoint operators, which for matrices is given by

$$\frac{d}{dt}U = -iAU$$

where A is selfadjoint operator. If we take the standard translation representation

$$U(h)f = f(x - h)$$

then

$$i\frac{d}{dh}U(h)f = -i\frac{d}{dx}U(h)f = (\frac{1}{i}\partial_x)U(h)f.$$

After a Fourier transform $\frac{1}{i}\partial_x$ becomes the multiplication by k. The spectral theorem says that selfadjoint operators are unitarily equivalent to a multiplication operator in the same fashion as above.

It is a basic principle of quantum mechanics that 'observables' are selfadjoint operators which play a central role in the formalism and interpretation of quantum mechanics. One of the most basic one is called $'x'$. In a translation invariant set there is the group of translations $U(h)$, with the obvious action on x:

$$U(-h)xU(h) = x + h1.$$

The Stone-von Neumann theorem classifies Hilbert spaces with such an action.

A particular case is the time translation. Stone's theorem relates it to a selfadjoint operator, which is called Hamilton operator.

One of the corner stones of quantum mechanics is a recipe how to construct Hamilton operators for the hull of atoms, and more complicated objects. On the side of mathematics this is the area of quantization, pseudodifferential operators and semiclassical analysis.

We will be brief on this recipe, and postpone its discussion and the discussion of symmetry groups to later chapters. This section is devoted to Stone's theorem, the spectrum and diagonalization of selfadjoint operators and unbounded operators. This will allow us to discuss the commutation relation

$$[x_j, -i\partial_{x_k}] = i\delta_{jk},$$

its relation to the Heisenberg group and Heisenberg's uncertainty relation. We will briefly touch upon the question of measurements and the interpretation of quantum mechanics.

3.1 The spectrum of continuous operators

Let X, Y be complex Banach spaces and $L(X,Y)$ be the space of continuous linear operators from X to Y with norm

$$\|T\|_{X\to Y} = \sup_{\|x\|_X \leqslant 1} \|Tx\|_Y.$$

Definition 3.1. *Let $T \in L(X,X)$. The* resolvent set $\rho(T)$ *consists of all $\lambda \in \mathbb{C}$ for which $T - \lambda 1$ is invertible. The complement is the* spectrum $\sigma(T)$.

Lemma 3.2. *Suppose that $T \in L(X,Y)$ is invertible. Then $T-S$ is invertible if $\|S\|_{X\to Y}\|T^{-1}\|_{Y\to X} < 1$. The map $T \to T^{-1}$ is analytic in the sense that we can expand it locally into a power series.*

Proof. We observe that, since $\|AB\|_{X\to X} \leqslant \|A\|_{X\to X}\|B\|_{X\to X}$we have $\|A^j\|_{X\to X} \leqslant \|A\|^j_{X\to X}$. Moreover

$$(T-S)T^{-1}\sum_{j=0}^{\infty}(ST^{-1})^j = 1_Y$$

and

$$T^{-1}\sum_{j=0}^{\infty}(ST^{-1})^j(T-S) = 1_X.$$

Convergence is immediate and hence

$$(T - S)^{-1} = T^{-1} \sum_{j=0}^{\infty} (ST^{-1})^j$$

which is the desired power series.

□

The theorem of the inverse operator, a consequence of the open mapping principle implies

Lemma 3.3. *$T \in L(X, Y)$ is invertible if*

1. *The null space is trivial*

2. *The range is closed*

3. *The closure of the range is Y.*

The dual operator $T' : Y^* \to X^*$ is defined by

$$T'y^*(x) = y^*(Tx).$$

It is invertible if and only if T is invertible.

Lemma 3.4. *The following statements are always true.*

1. *$\sigma(T) \subset \overline{B_R(0)}$ where $R = \|T\|_{X \to X}$.*

2. *$\sigma(T)$ is compact and nonempty.*

3. *$\sigma(T) = \sigma(T')$.*

4. *Let p be a polynomial. Then*

$$\sigma(p(T)) = p(\sigma(T)).$$

5. *$\sigma(T) \subset \overline{B_r(0)}$ where*

$$r = \liminf_{n \to \infty} \|T^n\|_{X \to X}^{1/n}.$$

$\sigma(T)$ is not contained in any smaller ball centers at 0.

Proof. Since

$$(T-z)(\sum_{j=0}^{\infty}(z-z_0)^j(T-z_0)^{-j-1} = 1$$

if T_{z_0} is invertible and $|z-z_0|$ small we obtain

$$\rho(T) \ni z \to x^*(T-z)^{-1}x$$

is holomorphic for all $x \in X$ and $x^* \in X^*$. Let $|\lambda| > R$. Then

$$(T-\lambda)\sum_{j=0}^{\infty}\lambda^{-j-1}T^j = -1_X = \sum_{j=0}^{\infty}\lambda^{-j-1}T^j(T-\lambda).$$

The sum converges since $|\lambda| > \|T\|_{X\to X}$ by assumption.

The set $\rho(T)$ is open by Lemma 3.2, hence $\sigma(T)$ is closed and bounded and hence compact. It is nonempty by the last part of the theorem.

We know from functional analysis that T is invertible if and only if T' is invertible. This implies the third statement.

Suppose that $\lambda \notin p(\sigma(T))$. By the fundamental theorem of algebra

$$p(z) - \lambda = c_0 \prod (z - z_j)$$

with $z_j \in \rho(T)$. Thus $T - z_j$ is invertible, and hence $\lambda \in \rho(p(T))$. Now assume that $\lambda \in p(\sigma(T))$. Then one of the z_j is in $\sigma(T)$. We assume that it is the first one. Either $T - z_1$ has a null space, and then $p(T) - \lambda$ has a null space, or the range is not the full space, in which case the range of $p(T) - \lambda$ is not the full space. Thus $p(T) - \lambda$ is not invertible and $\lambda \in \sigma(p(T))$.

Since

$$(\sigma(T))^j = \sigma(T^j) \subset B_{\|T^j\|}(0)$$

we obtain

$$\sigma(T) \subset \overline{B_r(0)}$$

with r as in the lemma. Now suppose that

$$\sigma(T) \subset \overline{B_a(0)}.$$

We will prove that then $a \geqslant r$, or more precisely

$$\limsup_{n\to\infty} \|T^n\|^{1/n} \leqslant a. \tag{3.1}$$

Let $x^* \in X^*$ and $x \in X$. The function

$$z \to x^*(1 - zT)^{-1}x \in \mathbb{C}$$

is holomorphic in $B_{1/a}(0)$ and, if z is small, then

$$(1-zT)^{-1} = \sum_{j=0}^{\infty} (zT)^j$$

by Part 1. Thus, for every $r' < 1/a$, by the residue theorem

$$x^* T^j x = \frac{1}{2\pi i} \int_{\partial B_{r'}(0)} x^* z^{-j-1} (1-zT)^{-1} x dz.$$

This is bounded by $c_{r'}(r')^{-j-1} \|x^*\|_{X*} \|x\|_X$ and hence

$$\|T^j\|_{X \to X} \leqslant c_{r'}(r')^{-j-1}, \quad \forall r' < 1/a,$$

which implies (3.1).

Similarly we prove that $\sigma(T)$ is not empty. Suppose it is empty. Then, by Lemma 3.2 as in part 1,

$$f(z) = x^*(T-z)^{-1} x$$

is holomorphic in $\mathbb{C}$. It is bounded and decays to zero as $|z| \to \infty$ by the proof of part 1. Hence

$$x^*(T-z)^{-1} x = 0$$

for all x^*, x and z (this follows from the residue theorem by

$$2\pi i f(z_0) = \lim_{R \to \infty} \int_{\partial B_R(z_0)} \frac{f(z)}{z - z_0} dz = 0.)$$

Thus $(T-z)^{-1} = 0$ which is absurd and a contradiction. □

[03.05.2017]

[05.05.2017]

3.2 The spectrum of normal operators I

In this section we only consider separable Hilbert spaces H with an inner product $\langle .,. \rangle$, which we assume to be complex linear in the first variable. The norm is given by $\|x\|_H^2 = \langle x, x \rangle$.

Definition 3.5. *Let $T \in L(H_1, H_2)$. Its adjoint $T^* \in L(H_2, H_1)$ is defined by*

$$\langle Tx, y \rangle_{H_2} = \langle x, T^* y \rangle_{H_1}.$$

We say that $T \in L(H,H)$ is normal if

$$T^*T = TT^*,$$

selfadjoint if $T = T^*$, positive semidefinite if in addition

$$\langle Tx, x\rangle \geqslant 0$$

and positive definite if there exists $\delta > 0$ so that in addition

$$\langle Tx, x\rangle \geqslant \delta \|x\|_H^2.$$

Lemma 3.6. *Suppose that T is normal. Then*

$$\|T^k\|_{H\to H} = \|T\|_{H\to H}^k.$$

As a consequence

$$\sup\{|\lambda| : \lambda \in \sigma(T)\} = \|T\|.$$

Proof.

$$\begin{aligned}
\|Tf\|_H^2 =& \langle Tf, Tf\rangle \\
=& \langle f, T^*Tf\rangle \\
\leqslant& \|T^*T\|_{H\to H}\|f\|_H^2
\end{aligned}$$

and hence (obviously $\|T^*T\| \leqslant \|T\|^2$)

$$\|T^*T\|_{H\to H} = \|T\|_{H\to H}^2.$$

Then

$$\begin{aligned}
\|T^2 f\|_H^2 =& \langle T^2 f, T^2 f\rangle \\
=& \langle Tf, T^*T^2 f\rangle \\
=& \langle Tf, TT^*Tf\rangle \\
=& \langle T^*Tf, T^*Tf\rangle \\
=& \|T^*Tf\|_H^2
\end{aligned}$$

and hence

$$\|T^2\| = \|T^*T\| = \|T\|^2$$

if T is normal. Similarly $\|T^{2k}\| = \|T^k\|^2$ and $\|T\|^{2^n} = \|T\|^{2^n}$. Since for any k there exist j, n such that $j + k = 2^n$ and hence

$$\|T\|^{2^n} = \|T^{2^n}\| \leqslant \|T^j\|\|T^k\| \leqslant \|T\|^j\|T\|^k = \|T\|^{2^n},$$

all inequalities above have to be equalities and hence $\|T^k\| = \|T\|^k$. The last statement follows now from Proposition 3.4.

□

Lemma 3.7. *Let T be normal.*

1. *T is selfadjoint if and only if $\sigma(T) \subset \mathbb{R}$.*
2. *T is positive semidefinite iff $\sigma(T) \subset [0, \infty)$.*
3. *T is positive definite iff $\sigma(T) \subset (0, \infty)$.*

Proof. Let T be selfadjoint and $A = 1 + iT$. Then

$$(x, y) \to \langle Ax, y\rangle = \langle x, y\rangle + i\langle Tx, y\rangle$$

is a continuous bilinear form, linear in the first argument, and antilinear in the second. Moreover, since by selfadjoint property $\langle Tx, x\rangle = \langle x, Tx\rangle = \overline{\langle Tx, x\rangle} \in \mathbb{R}$, we have

$$\mathrm{Re}\langle Ax, x\rangle = \|x\|_H^2.$$

By the Lemma of Lax Milgram A is invertible. For any $\lambda = a + ib$ with $b \neq 0$, we know that the operator $b^{-1}(T - a)$ is selfadjoint and the operator

$$-ib^{-1}(\lambda - T) = 1 + ib^{-1}(T - a)$$

is invertible and hence $\lambda \in \rho(T)$. Therefore $\sigma(T) \subset \mathbb{R}$.

Now let T be normal and $\sigma(T) \subset \mathbb{R}$. Then for all $t \in \mathbb{R}\backslash\{0\}$, $T - it$ is invertible with $\sigma(T - it) \subset (\mathbb{R} - it)$. We claim that

$$\sigma\big((T - it)^{-1}\big) = (\sigma(T) - it)^{-1}. \tag{3.2}$$

This follows from the trivial observation that if T and $T - \lambda$ are invertible with $\lambda \neq 0$, then $T^{-1} - \lambda^{-1}$ is invertible since $\lambda T(T^{-1} - \lambda^{-1}) = \lambda - T$ and hence

$$(\lambda - T)^{-1}\lambda T(T^{-1} - \lambda^{-1}) = 1 = (T^{-1} - \lambda^{-1})\lambda T(\lambda - T)^{-1}.$$

Moreover T^{-1} is normal if T is normal and invertible.

Using the claim (3.2) we get by Lemma 3.6

$$\|(T - it)^{-1}x\| \leqslant |t|^{-1}\|x\|, \text{ that is, } \|(T - it)x\| \geqslant |t|\|x\|$$

and hence

$$0 \leqslant \|(T - it)x\|^2 - t^2\|x\|^2 = \|Tx\|^2 - 2t\,\mathrm{Im}\langle Tx, x\rangle$$

for all t. Thus $\mathrm{Im}\langle Tx, x\rangle = 0$ and hence

$$\langle Tx, x\rangle = \langle x, Tx\rangle \in \mathbb{R}.$$

Then

$$\langle (T - \frac{1}{2}(T + T^*))x, x\rangle = 0$$

for all x where $T + T^*$ is selfadjoint. Similarly $S = i(T - T^*)$ is selfadjoint and it satisfies

$$\langle Sx, x\rangle = 0$$

for all $x \in H$. We claim that then $S = 0$ since

$$\langle Sx, y\rangle = \frac{1}{4}\Big(\big\langle S(x+y), x+y\big\rangle - \big\langle S(x-y), x-y\big\rangle\Big) = 0$$

for all $x, y \in H$.

Now suppose that T is positive semidefinite and $\lambda < 0$. We apply the same argument to $A = T - \lambda$.

Suppose that $\sigma(T) \subset [0, \infty)$. Then T is selfadjoint by the previous step. If $t > 0$ then in the same ways as above

$$\|(t + T)x\| \geqslant t\|x\|$$

and

$$0 \leqslant \|(t + T)x\|^2 - t^2\|x\|^2 = \|Tx\|^2 + 2t\langle Tx, x\rangle$$

and hence $\langle Tx, x\rangle \geqslant 0$.

The last statement about positive definite operators follows by adding a multiplie of the identity from the positive semidefinite case.

□

Lemma 3.8. *Let p be a polynomial and T be normal. Then $p(T)$ is normal. If T is selfadjoint and p is real then $p(T)$ is selfadjoint. If p is real and nonnegative on $\sigma(T)$ then $p(T)$ is positive semidefinite.*

Proof. An easy computation shows that T^k is normal if T, and selfadjoint if T is selfadjoint. Since $\sigma(p(T)) = p(\sigma(T))$ the last statement follows from the previous lemma. □

Theorem 3.9 (Stone-Weierstraß)**.** *Let $K \subset \mathbb{R}^d$ be compact and $f \in C(K; \mathbb{R})$. Then there exists a sequence of polynomial p_n in d variables so that*

$$\|f - p_n\|_{C_b(K)} \to 0.$$

Theorem 3.10. *Let T be selfadjoint with spectrum $K = \sigma(T)$. Then there is a unique isometry*

$$\phi : C(K; \mathbb{R}) \ni f \to f(T) \in L(X, X)$$

so that the range consists of selfadjoint operators and

$$\phi(x) = T$$

$$\phi(fg) = \phi(f)\phi(g).$$

Moreover

$$\sigma(\phi(f)) = f(\sigma(T)).$$

This theorem defines a so-called operator calculus which may be considered as 'spectral theorem' resp. a diagonalization of T. We can easily extend the theorem to complex valued functions by splitting real and imaginary parts. We will write

$$f(T) := \phi(f).$$

Proof. For monomials we must have

$$\phi(x^n) = T^n$$

if there is a map with these properties. Hence we define ϕ on polynomials by

$$\phi(p) = p(T)$$

which is clearly selfadjoint and satisfies all the properties for real polynomials. Let $f \in C(K;\mathbb{R})$ and p_n a sequence of polynomials converging uniform in K to f. Then

$$\sigma(\phi(p_n - p_m)) = \sigma(p_n(T) - p_m(T)).$$

By Lemma 3.6

$$\begin{aligned} \|\phi(p_n) - \phi(p_m)\|_{L(X,X)} &= \|(p_n - p_m)(T)\| \\ &= \sup\{|\lambda| : \lambda \in \sigma((p_n - p_m)(T))\} \\ &\leqslant \sup_{y \in K} |p_n(y) - p_m(y)| \to 0. \end{aligned}$$

We define

$$f(T) = \lim_{n\to\infty} p_n(T).$$

Uniqueness and the properties are immediate consequences. $\square$

It is not hard to extend this theorem to normal operators. However, we will obtain a more general result later anyhow.

[05.05.2017]

[10.05.2017]

3.3 Orthogonal polynomials. Favard's theorem

We will attempt to obtain a more precise 'spectral' theorem, for which we will use the theory of orthonormal polynomials, which is interesting in its own right.

Let μ be a Radon measure on $\mathbb{R}$ with $|x|^N \in L^2(\mu)$ for all N and $\mu(\mathbb{R}) = 1$. We call μ trivial if it is a finite sum of Dirac measures. In the sequel we assume that μ is nontrivial. Notice that

$$x^k = \sum_{j=0}^{k-1} a_j x^j, \qquad \text{in } L^2(\mu)$$

for some a_j if and only if μ is trivial - if the identity holds in $L^2(\mu)$ then it holds almost everywhere. Then for finitely many points one obtains a Vandermonde matrix applied to the vectors $((a_j), 1)$, which can only be zero if there are less than k points.

We use the Gram-Schmidt procedure to orthogonalize the sequence x^k and obtain the monic orthogonal polynomials

$$P_n(x) = x^n + \sum_{j=0}^{n-1} a_j x^j,$$

$$P_0 = 1, P_1 = x - \int_{\mathbb{R}} x d\mu, \dots .$$

and the orthonormal polynomials

$$p_n = \|P_n\|^{-1}_{L^2(\mu)} P_n.$$

We define

$$a_n = \frac{\|P_n\|_{L^2(\mu)}}{\|P_{n-1}\|_{L^2(\mu)}} > 0,$$

so that

$$\|P_n\|_{L^2(\mu)} = \prod_{j=1}^n a_j.$$

Lemma 3.11. *There exist b_n so that*

$$xP_n(x) = P_{n+1}(x) + b_{n+1}P_n(x) + a_n^2 P_{n-1}(x)$$

with $b_n \in \mathbb{R}$. Then

$$xp_n(x) = a_{n+1}p_{n+1} + b_{n+1}p_n + a_n p_{n-1}. \tag{3.3}$$

Proof. By construction the P_n are orthogonal to all polynomials of degree $< n$. If $j < n-1$ then

$$\langle P_j, xP_n\rangle = \langle xP_j, P_n\rangle = 0$$

and hence there exist α, β and γ so that

$$xP_n(x) = \alpha P_{n+1}(x) + \beta P_n(x) + \gamma P_{n-1}(x).$$

Sicne xP_n and P_{n+1} are monic we have $\alpha = 1$. In particular

$$\langle xP_n, P_{n+1}\rangle = \|P_{n+1}\|^2$$

and

$$\gamma = \langle xP_n, P_{n-1}\rangle / \|P_{n-1}\|^2 = \|P_n\|^2/\|P_{n-1}\|^2 = a_n^2.$$

Thus

$$\beta = \langle xP_n, P_n\rangle / \|P_n\|^2 := b_{n+1} \in \mathbb{R}$$

and finally

$$xp_n(x) = \frac{\|P_{n+1}\|}{\|P_n\|} p_{n+1} + b_{n+1} p_n(x) + a_n^2 \frac{\|P_{n-1}\|}{\|P_n\|} p_{n-1}$$

which gives (3.3). □

The Jacobi matrix is defined to be

$$J = \begin{pmatrix} b_1 & a_1 & 0 & 0 & \dots \\ a_1 & b_2 & a_2 & 0 & \dots \\ 0 & a_2 & b_3 & a_3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Lemma 3.12. *Suppose that μ is supported on a compact interval. Let*

$$\eta = 2 \sup |a_n| + \sup |b_n|.$$

Then $\operatorname{supp} \mu \subset [-\eta, \eta]$ *and, if* $\operatorname{supp} \mu \subset [-R, R]$ *then* $\eta \leqslant 3R$.

Proof. The span of the $p_n(x)$ is dense in $L^2(\mu)$ by the theorem of Stone-Weierstrass 3.9 and the density of continuous functions in $L^2(\mu)$ since μ is a compactly supported Radon measure.

The multiplication by x can be expressed through the matrix J. In particular, if $f = \sum_{j=1}^{\infty} p_{j-1}(x)$ then

$$xf = \sum_{j=1}^{\infty} (a_j p_j + b_j p_{j-1} + a_{j-1} p_{j-2})$$

hence

$$\|xf\|_{L^2(\mu)} \leqslant \eta \|f\|_{L^2(\mu)}.$$

In particular

$$\left| \int_{\mathbb{R}} x^n d\mu \right| \leqslant \|x^n\|_{L^2(\mu)} \leqslant \eta^n.$$

But this implies that μ is supported in $[-\eta, \eta]$. Now suppose that μ is supported in $[-R, R]$. By construction

$$b_{n+1} = \langle xp_n, p_n \rangle, \quad a_{n+1} = \langle xp_n, p_{n+1} \rangle$$

and hence $0 < a_n \leqslant R$, $|b_n| \leqslant R$. □

Theorem 3.13 (Favard's theorem)**.** *Let (a_n) be a nonnegative bounded sequence, and let (b_n) be a bounded sequence. Then there exists a unique probability measure so that (a_n, b_n) are the Jacobi parameters, i.e. entries of its Jacobi matrix.*

Proof. We first prove uniqueness. Let μ and ν be such probability measures. Two measures are equal if

$$\int f d\mu = \int f d\nu$$

for every continuous function. By the Stone-Weierstraß approximation theorem 3.9 polynomials are dense in the continuous functions and hence it suffices to prove

$$\int x^n d\mu = \int x^n d\nu. \tag{3.4}$$

This holds for $n = 0$ and suppose this also holds for $n \leqslant k - 1$. Since the a_n and b_n determine P_k by $xP_{k-1} - b_k P_{k-1} - a_{k-1}^2 P_{k-2}$, we have

$$\int P_k d\mu - \int P_k d\nu = 0$$

by the orthogonality to 1.

Existence is more involved. Let J_n be the upper left $n \times n$ block of J and let P_n be the monic polynomial corresponding to J_n.

Lemma 3.14. 1. *All roots of P_n are real and simple.*

2. *The roots of P_n and P_{n-1} are interlaced.*

Proof. If $P_n(y) = 0$ then

$$P_{n+1}(y) + a_n^2 P_{n-1}(y) = 0$$

and $P_{n+1}(y)$ and $P_{n-1}(y)$ have opposite signs. Now we do induction on n. Suppose the lemma holds for P_k for $k \leqslant n$. Let y_j be the ordered zeros of P_n. Then $P_{n-1}(y_j)$ has a different sign at two adjacent zeros of P_n, and the same is true for P_{n+1}. Checking $x \to \pm\infty$ one sees that P_{n+1} has one zero in each of the intervals $(-\infty, y_1), (y_1, y_2) \dots (y_n, \infty)$. Hence it has $n+1$ real zeros which have to be simple since the degree of P_{n+1} is $n+1$, and interlaced. $\square$

Theorem 3.15. *Let J_n, P_j^n and p_j^n be as above.*

1. *$p_n(y_j) = 0$ iff y_j is an eigenvalue of J_n. Then the vector*

$$\phi^j = (\phi_k^j)_{1 \leqslant k \leqslant n} = \left(\frac{p_{k-1}(y_j)}{\left(\sum_{l=1}^n |p_{l-1}(y_j)|^2 \right)^{\frac{1}{2}}} \right)_{1 \leqslant k \leqslant n} \tag{3.5}$$

   is the eigenvector of J_n associated to the eigenvalue y_j:

$$(J_n - y_j)\phi^j = 0.$$

2. *For $j \neq k$ $\sum\limits_{m=1}^{n} \phi_m^j \overline{\phi_m^k} = 0$.*

3. *Let $\mu_n = \sum_{j=1}^n |\phi_1^j|^2 \delta_{y_j}$. Then J_n is the Jacobi matrix of μ_n.*

4. $\det(z - J_n) = P_n(z)$.

Proof. Equation (3.3) implies that

$$J_n(p_{m-1}(y_j))_{1 \leqslant m \leqslant n} = y_j (p_{m-1}(y_j))_{1 \leqslant m \leqslant n}$$

for all zeros y_j of p_n. Since p_n has n simple zeros, the y_j, $1 \leqslant j \leqslant n$ are simple eigenvalues of $n \times n$ matrix J_n with the eigenvectors ϕ^j of the theorem.

Since J_n is real and symmetric and hence selfadjoint, the eigenvectors are orthogonal and real: $\delta_{jk} = \langle \phi^j, \phi^k \rangle = \sum_{m=1}^n \overline{\phi_m^j} \phi_m^k$.

By (3.5)

$$\phi_m^j = (p_{m-1}(y_j))\phi_1^j$$

hence

$$\delta_{jk} = \sum_{m=1}^{n} \overline{\phi_m^j} \phi_m^k = \sum_{m=1}^{n} \overline{\phi_1^j} \phi_1^k \overline{p_{m-1}(y_j)} p_{m-1}(y_k).$$

We read this as saying that a product of two $n \times n$ matrices is the identity. Then also

$$\delta_{jk} = \sum_{m=1}^{n} \overline{\phi_1^m} \phi_1^m \overline{p_{k-1}(y_m)} p_{j-1}(y_m) = \int p_{j-1} p_{k-1} d\mu_n.$$

Thus the (p_j) are orthonormal polynomials with respect to μ_n.

Statement 1 implies

$$\det(x - J_n) = P_n(x)$$

since both polynomials have the same zeros and both are monic.

$\square$

[10.05.2017]

[12.05.2017]

We continue with the proof of Theorem 3.13. Now let μ_n be the measures of Theorem 3.15. Then

$$\int 1 d\mu_n = \int 1 d\mu_m = 1$$

and

$$\int p_j d\mu_n = \int p_j d\mu_m = 0$$

for $1 \leqslant j < n \leqslant m$. Thus $\int x^l d\mu_n$ is independent of n provided $n > l$ and the limit

$$\lim_{n \to \infty} \int x^j d\mu_n$$

exists and defines an element in the dual space of $C_b([-\eta, \eta])$, and hence a unique measure with the desired properties. $\square$

3.4 The spectrum of selfadjoint operators: the second version

Let H be an infinite dimensional Hilbert space and $T \in L(H)$ be selfadjoint. We call $\phi \in H$ with $\|\phi\| = 1$ cyclic if the span of $(T^j \phi)_{0 \leqslant j}$ is dense in H.

Theorem 3.16. *Let T be selfadjoint and ϕ be cyclic. Then there exists a unique compactly supported probability measure μ on $\mathbb{R}$ and a unique unitary map $U : L^2(\mu) \to H$ so that*

$$TUf = Uxf$$

and

$$U1 = \phi.$$

Proof. We apply the orthogonalization procedure to $T^n\phi$ (linearly independent since ϕ is cyclic, and the dimension is ∞) to obtain Φ_n in the form

$$\Phi_n = T^n\phi + \sum_{j=0}^{n-1} c_j T^j \phi$$

so that

$$\langle \Phi_n, \Phi_m \rangle = \delta_{nm}.$$

Then $T\Phi_k$ is in the span of $(\Phi_m)_{m \leqslant k+1}$. In particular

$$\langle \Phi_l, T\Phi_k \rangle = 0$$

if $l > k+1$. Thus $|j-m| > 1$ implies $\langle \Phi_j, \Phi_m \rangle = 0$ and the (infinite) matrix of T in this basis is tridiagonal. We write

$$T\Phi_n = \alpha \Phi_{n+1} + \beta \Phi_n + \gamma \Phi_{n-1}$$

and define

$$a_n = \|\Phi_n\| / \|\Phi_{n-1}\|.$$

Let $\phi_n = \Phi_n / \|\Phi_n\|$. Then

$$T\phi_n = a_{n+1}\phi_{n+1} + b_{n+1}\phi_n + a_n \phi_{n-1} \tag{3.6}$$

and

$$b_{n+1} = \langle T\phi_n, \phi_n \rangle, a_{n+1} = \langle T\phi_n, \phi_{n+1} \rangle.$$

Both are bounded by $\|T\|$. We apply Favard's theorem: There exists a unique measure μ and a sequence of orthonormal polynomials analogous to the ϕ_n. We define U by

$$Up_n = \phi_n.$$

This is clearly unitary, $Ux^n = \Phi^n = T^n\phi$ for $1 \leqslant n$ and hence $U(xf) = TUf$. □

Theorem 3.17. *Let T be selfadjoint. There exists measure on $\mathbb{R} \times \mathbb{N}$ supported on $K \times \mathbb{N}$ for some $K = \sigma(T)$ and a unitary map $U \in L(L^2(\mathbb{R} \times \mathbb{N}); H)$ so that*

$$Uxf = TUf.$$

Proof. We claim that there exists a finite or infinite ONS sequence (ϕ_m) so that

$$\langle T^k \phi_m, \phi_n \rangle \neq 0$$

unless $m = n$ and the span of $(T^k\phi_m)_{m,k}$ is dense in H. We then apply the previous theorem for all $H_m = \overline{\text{span}\{T^k\phi_m : k \geqslant 0\}}$. We assume that all H_m are infinite dimensional. The arguments are easily modified in the finite dimensional case. Since $T : H_m \to H_m$ we obtain the theorem.

Let $(\tilde{\phi}_j)$ be a basis. We choose $\phi_1 = \tilde{\phi}_1$ and

$$H_1 = \overline{\text{span}\{T^k\phi_1 : k \geqslant 0\}}.$$

Let $\tilde{\phi}_j$ be the first j so that $\tilde{\phi}_j \notin H_1$. We project it to $H_1^\perp$ and normalize it and denote it by ϕ_2. We obtain the H_m recursively. □

It is not hard to see that the spectrum of a multiplication operator by a continuous function f on $L^2(\mu)$ is the image of the support of μ under f.

Corollary 3.18 (Borel functional calculus)**.** *Let T be selfadjoint, K its spectrum. Let $\mathcal{B}(K)$ be the set of bounded Borel measurable functions on K with the standard norm. Then there is a unique algebra morphism*

$$\Psi : \mathcal{B}(K) \to L(H)$$

so that

$$\Psi(x^n) = T^n$$

for $0 \leqslant n$.

Proof. This is trivial for a multiplication operator. By Theorem 3.17 it suffices to consider a multiplication operator. We postpone the proof of uniqueness (it follows from the argument in Lemma 3.21 below). □

Definition 3.19. *Let T be selfadjoint. We define the* spectral resolution *as the family of projection operators*

$$P(t) = \Psi(\chi_{(-\infty,t]}) := \chi_{(-\infty,t]}(T).$$

Then $P(t) = 0$ if $t < -\|T\|$, $P(t) = 1$ if $t \geqslant \|T\|$ and

$$P(t)P(s) = P(\min\{t, s\})$$

Moreover $P^*(t) = P(t)$ and the $P(t)$ are selfadjoint and positive semidefinite.

3.5 The spectrum of normal operators II

Let T_j, $j = 1, \cdots, N$ be a set of commuting selfadjoint operators:

$$T_i T_j = T_j T_i.$$

We call $\phi \in H$ cyclic, if $\|\phi\| = 1$ and the span of

$$(T_i^k \phi)_{i,k}$$

is dense in H.

Theorem 3.20. *Suppose that ϕ is cyclic. Then there exists a unique probability measure μ on*

$$\bigtimes_{j=1}^{N} [-\|T_j\|, \|T_j\|]$$

and a unitary map $U : L^2(\mu) \to H$ so that

$$T_j U h = U x_j h, \qquad U1 = \phi.$$

Proof. As in the single operator case uniqueness of μ follows from

$$\langle \phi, T^\alpha \phi \rangle = \int x^\alpha d\mu_\phi.$$

Lemma 3.21. *Let T_1 and T_2 be commuting bounded selfadjoint operators and let f, g be bounded Borel functions. Then $f(T_1)$ and $g(T_2)$ commute.*

We use the notation

$$[T_1, T_2] = T_1 T_2 - T_2 T_1$$

for the commutator.

Proof. This is clear for polynomials, hence also for continuous functions f and g. Let f and g be Borel measurable and f_n, g_n continuous, uniformly bounded, with $f_n \to f$ and $g_n \to g$, μ_{T_1} and μ_{T_2} almost everywhere with the measures of Theorem 3.17. Then for all $h \in L^2(\mu_{T_1})$

$$f_n h \to f h$$

in $L^2(\mu_{T_1})$ by the convergence theorem of Lebesgue. Thus

$$0 = [f_n(T_1), g_m(T_2)]\psi \to [f(T_1), g_m(T_2)]\psi \qquad \text{as } n \to \infty$$

for all $\psi \in H$ and

$$0 = [f(T_1), g_m(T_2)]\psi \to [f(T_1), g(T_2)]\psi \qquad \text{as } m \to \infty$$

by the same argument. □

We define a measure μ on rectangles $R = \times_{j=1}^{N}(x_j, y_j]$

$$\mu(R) = \langle \phi, \prod_{j=1}^{N} \chi_{(x_j,y_j]}(T_j)\, \phi \rangle.$$

Then by Corollary 3.18, μ is supported on $\times_{j=1}^{N}[-\|T_j\|, \|T_j\|]$.

Lemma 3.22. $0 \leqslant \mu(R) \leqslant 1$. *It defines an outer measure which coincides with μ on rectangles.*

Proof. By Lemma 3.21, the operators $\chi_{(x_j,y_j]}(T_j)$ commute. Moreover the operator $\chi_{(x_j,y_j]}(T_j)$ is positive semidefinite, and thus $0 \leqslant \mu(R)$. If $R \subset R'$ then $\mu(R) \leqslant \mu(R')$ and $\mu(\mathbb{R}^N) = 1$. As for the Lebesgue measure this defines a premeasure on finite union of cubes, an outer measure on all sets, and a measure on Borel sets, which coincides with μ on rectangles and we denote this outer measure still by μ. □

We define U by

$$U \prod_{j=1}^{N} \chi_{(a_j,b_j]}(x_j) = \prod_{j=1}^{N} \chi_{(a_j,b_j]}(T_j)\phi$$

which extends to a linear and unitary map from $L^2(\mu)$ to H. By an approximation by step functions

$$Ux_j = T_j\phi$$

and hence $Ux^\alpha = T^\alpha\phi$ for every multiindex. This implies

$$U(x_j f) = T_j U(f)$$

for all $f \in L^2(\mu)$.

□

Theorem 3.23 (Normal operators)**.** *Let T be normal operator. Then there exists a measure μ on $\overline{B^{\mathbb{C}}_{\|T\|}(0)} \times \mathbb{N}$ and a unitary operator U so that*

$$Uz\psi = TU\psi$$

$$U\bar{z}\psi = T^*U\psi.$$

Proof. We write $T = T_1 + iT_2$ with $T_1 = \frac{1}{2}(T + T^*)$, $T_2 = \frac{1}{2i}(T - T^*)$ being selfadjoint operators. We have $(T_1 + iT_2)^* = T_1 - iT_2$ and

$$\begin{aligned} T_1^2 + T_2^2 - i[T_1, T_2] = (T_1 + iT_2)(T_1 - iT_2) = TT^* \\ T^*T = (T_1 - iT_2)(T_1 + iT_2) = T_1^2 + T_2^2 + i[T_1, T_2]. \end{aligned}$$

Thus T is normal iff T_1 and T_2 commute. It suffices to consider the case when there is a cyclic ϕ. Then there is a unique measure μ with compact support on $\mathbb{R}^2$ and a unitary map $U : L^2(\mu) \to H$ so that

$$U1 = \phi, \quad U(x_1 f) = T_1 U f, \quad U(x_2 f) = T_2 U f.$$

Thus

$$U((x_1 + ix_2)f) = (T_1 + iT_2)Uf = TUf$$

and

$$U((x_1 - ix_2)f) = (T_1 - iT_2)Uf = T^*Uf.$$

Again

$$\operatorname{supp} \mu = \sigma(M_z) = \sigma(T) \subset \overline{B_{\|T\|}(0)} \subset \mathbb{C}.$$

□

3.6 Unbounded selfadjoint operators

Given $h \in \mathbb{R}$ we define $S(h) \in L(L^2(\mathbb{R}))$ by

$$S(h)f(x) = f(x - h), \quad \forall f \in L^2(\mathbb{R}).$$

The operator S is unitary and satisfies

$$S(0) = 1, \qquad S(h_1 + h_2) = S(h_1)S(h_2) \qquad \text{for } h_1, h_2 \in \mathbb{R}.$$

It is not difficult to see that whenever $h \neq 0$

$$\|S(h) - S(0)\|_{L^2 \to L^2} = 2$$

and hence $h \to S(h) \in L(L^2(\mathbb{R}))$ is not continuous in the operator norm. We call a map $h \to T(h) : \mathbb{R} \to L(H)$ strongly continuous if

$$h \to T(h)\phi$$

is continuous from $\mathbb{R}$ to H for every $\phi \in H$. It is not hard to see that $h \to S(h)$ is strongly continuous, by use of the density of the compacted supported continuous functions in $L^2(\mathbb{R})$.

The 'generator' (to be defined later) of the translations is $-i\partial_x$, which is not a bounded operator. We want to establish a theory which says that every (one parameter) unitary group of operators (assuming strong continuity) has a selfadjoint generator.

Definition 3.24. *A densely defined (or unbounded) operator T on a Hilbert H is* a pair *consisting of* *a dense subspace $D(T)$* *and* *a linear map T* $: D(T) \to H$. *Its graph*

$$\Gamma(T) = \{(x, Tx) \in D(T) \times H\}$$

is a subspace of $H \times H$.

We write $S \subset T$ if $D(S) \subset D(T)$ and $T|_{D(S)} = S$.

We call it symmetric if

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

for all $\phi, \psi \in D(T)$. We call it closed if $\Gamma(T)$ is closed and closable if $\overline{\Gamma(T)}$ is the graph of an operator which is called closure.

Let T be an unbounded operator. Its adjoint T^* is defined by

$$\langle T\phi, \psi \rangle = \langle \phi, T^*\psi \rangle, \quad \forall \phi, \psi \in H$$

with

$$D(T^*) = \{\eta : \text{ there exists } c \text{ so that } |\langle T\phi, \eta \rangle| \leqslant c\|\phi\| \text{ for all } \phi \in D(A)\}.$$

We call T selfadjoint if $T^* = T$.

Lemma 3.25. *Let μ be a Radon measure on $\mathbb{R}^d$, F a Borel measurable function. We define*

$$D(T) = \Big\{ f : \int_{\mathbb{R}^d} F^2 |f|^2 d\mu < +\infty \Big\},$$

and

$$Tf = Ff, \quad \forall f \in D(T).$$

Then T is selfadjoint and closed.

Proof. We claim that the graph is closed: Let $f_n \in D(T)$ so that f_n and Ff_n are Cauchy sequences and $f = \lim\limits_{n\to\infty} f_n$. Then $Ff_n \in L^2$ and $Ff = \lim_{n\to\infty} Ff_n \in L^2$ and hence $f \in D(T)$.

If there exists c such that

$$\left| \int_{\mathbb{R}^d} F\phi\eta d\mu \right| \leqslant c\|\phi\|_{L^2}$$

for all ϕ with $F\phi \in L^2$ then $F\eta \in L^2$ and hence $D(T^*) = D(T)$. Symmetry is obvious. □

Lemma 3.26. *Suppose that T is a densely defined operator on H and that for some $\varepsilon > 0$*

$$\|T\phi\| \geqslant \varepsilon\|\phi\|.$$

Then T is closed iff the range is closed.

Proof. Exercise. $\square$

Definition 3.27. *Let T be a closed operator. We define $\rho(T)$ as the set of all z for which there exists a bounded operator S with range contained in $D(T)$ so that*

$$(T-z)S\phi = \phi \qquad \text{for all } \phi \in H$$

and

$$S(T-z)\phi = \phi \qquad \text{for all } \phi \in D(T).$$

The complement $\sigma(T) = \mathbb{C}\backslash\rho(T)$ is called spectrum.

[19.05.2017]

[24.05.2017]

Let T be symmetric. For $z \in \mathbb{C}\backslash\mathbb{R}$ we define the deficiency index

$$d(z) = \dim(\operatorname{Ran}(T-z))^{\perp} = \dim\ker(T^* - \bar{z}).$$

Example: $H = L^2([0,1])$, $D(T) = H_0^1([0,1])$, $T = -i\partial_x$. This operator is symmetric. The adjoint operator T^* has domain $H^1([0,1])$. To determine $d(i)$ we search for functions in $D(T^*)$ which satisfy

$$\phi \in \ker(T^* + i) \text{ i.e. } -i\partial_x\phi = -i\phi.$$

This is $\phi = ce^x \in H^1([0,1])$ which is not in $H_0^1([0,1])$ and $d(i) = 1$.

Theorem 3.28. *Let T be closed and symmetric. Then there are two non-negative integers $d_\pm$ so that $d(z) = d_\pm$ for $\pm \operatorname{Im} z > 0$. If $\langle T\phi, \phi\rangle \geqslant 0$ for $\phi \in D(T)$ then also $d_+ = d_-$.*

Proof. Let $\operatorname{Im} z > 0$. We will show that there exists a ball around z so that $d(z)$ is constant on that ball. Together with a similar argument for $T \geqslant 0$ this completes the proof.

Suppose that V, W are closed subspaces of H. If $V \cap W = \{0\}$ then

$$\dim V \leqslant \dim W^{\perp}.$$

We apply this with $W = \operatorname{Ran}(T-z)$ and $V = \ker(T^* - \bar{w})$ with $|z-w| < \operatorname{Im} z/2$. It suffices to prove that $V \cap W = \{0\}$. Let $\eta \in V \cap W$. There exists

$\phi \in D(T)$ so that $\eta = (T - z)\phi$ and $(T^* - \bar{w})\eta = 0$ and hence $(T^* - \bar{z})\eta = (\bar{w} - \bar{z})\eta$. Thus

$$\|\eta\|^2 = \langle (T - z)\phi, \eta\rangle = \langle \phi, (T^* - \bar{z})\eta\rangle = (w - z)\langle \phi, \eta\rangle$$

and hence

$$\|\eta\|^2 \leqslant |w - z|\|\eta\|\|\phi\| \leqslant \frac{|w - z|}{\operatorname{Im} z}\|\eta\|^2,$$

thus $\eta = 0$. Here we use that

$$\operatorname{Im}\langle (T - z)\phi, \phi\rangle = -\operatorname{Im} z\|\phi\|^2$$

and hence

$$\|\eta\| = \|(T - z)\phi\| \geqslant |\operatorname{Im} z|\|\phi\|$$

for $\phi \in D(T)$. The second part is similar. □

Theorem 3.29. *Let T be a closed symmetric operator. Then T is selfadjoint iff $d_+ = d_- = 0$.*

Proof. Suppose first that $T = T^*$. If $(T^* - \bar{z})\phi = 0$ with $\operatorname{Im} z \neq 0$ then

$$z\|\phi\|^2 = \langle \phi, T^*\phi\rangle = \langle T\phi, \phi\rangle \in \mathbb{R}$$

which implies $d_\pm = 0$.

Now assume that $d_\pm = 0$. Given $\phi \in D(T^*)$ we find $\eta \in D(T)$ with

$$(T + i)\eta = (T^* + i)\phi.$$

Since $T \subset T^*$

$$(T^* + i)(\eta - \phi) = (T + i)\eta - (T^* + i)\phi = 0$$

and $\eta - \phi \in \ker(T^* + i)$ and hence $\phi = \eta \in D(T)$. Thus $D(T) = D(T^*)$ and $T = T^*$. □

Definition 3.30. *Let T be closed and symmetric. The* Cayley transform *is*

$$U\psi = \begin{cases} (T - i)(T + i)^{-1}\psi & \text{if } \psi \in \operatorname{Ran}(T + i) \\ 0 & \text{if } \psi \in \operatorname{Ran}(T + i)^\perp = \ker(T^* - i) \end{cases}.$$

Theorem 3.31. *Suppose that T is a closed symmetric operator and U its Cayley transform.*

- *U is an isometry from* $\operatorname{Ran}(T + i)$ *to* $\operatorname{Ran}(T - i)$.

- *T is selfadjoint iff U is unitary.*
- *ϕ is cyclic for U if and only if it is cyclic for $(T+i)^{-1}$.*
- *For U unitary, $U\phi = \phi$ has only trivial solutions.*

Proof. If $(T+i)\phi = \psi$ then

$$\|\psi\| = \|(T+i)\phi\| = \|(T-i)(T+i)^{-1}\psi\|$$

since

$$\|(T+i)\phi\|^2 = \|T\phi\|^2 + \|\phi\|^2 = \|(T-i)\phi\|^2.$$

Thus $U|_{\mathrm{Ran}(T+i)}$ is an isometry to $\mathrm{Ran}(T-i)$. Surjectivity holds since we can argue in the same fashion with $(T+i)(T-i)^{-1}$.

U is unitary if T is selfadjoint.

The third part follows from

$$U = 1 - 2i(T+i)^{-1}.$$

If $U\phi = \phi$ then $\|U\phi\| = \|\phi\|$, $\phi \in \mathrm{Ran}(T+i)$, and $U^*\phi = U^*U\phi = \phi$. For $\eta \in D(T)$

$$\begin{aligned} 0 = \langle (T+i)\eta, (U^*-1)\phi\rangle &= \langle (U(T+i) - (T+i))\eta, \phi\rangle \\ &= \langle ((T-i) - (T+i))\eta, \phi\rangle = -2i\langle \eta, \phi\rangle \end{aligned}$$

and hence $\phi \in D(T)^\perp = \{0\}$. □

Theorem 3.32 (Spectral theorem for unbounded selfadjoint operators)**.** *Suppose that T is a unbounded selfadjoint operator on H. Then there is a Radon measure μ on $\mathbb{R} \times \mathbb{N}$ and an isometry*

$$U : L^2(\mu) \to H,$$

so that $U : D(M_x) \to D(T)$ is bijective and that if $xf \in L^2(\mu)$ then $U(f) \in D(T)$ and

$$U(xf) = TU(f).$$

Proof. Let V be the Cayley transform of T. It is unitary and hence bounded and normal. By Theorem 3.23 there is a Radon measure $\tilde\mu$ on $\mathbb{C} \times \mathbb{N}$ and a unitary map

$$\tilde U : L^2(\tilde\mu) \to H$$

so that

$$\tilde U z\tilde f = V\tilde U\tilde f, \quad \tilde U\bar z\tilde f = V^*\tilde U\tilde f.$$

Since V is unitary, its spectrum is contained in the unit circle and hence the support of $\tilde{\mu}$ is contained in the unit circle with $\tilde{\mu}(\{1\} \times \mathbb{N}) = 0$.

Let $\phi(z) = i\frac{1+z}{1-z}$ so that $\phi(z) \in \mathbb{R}$ if $|z| = 1$, $z \neq 1$. The multiplier operator M_ϕ defines a selfadjoint operator on $L^2(\tilde{\mu})$ with dense domain since $\tilde{\mu}(\{1\} \times \mathbb{N}) = 0$. Let $\tilde{f} \in D(M_\phi)$ and

$$\tilde{g} = \phi(z)\tilde{f} = i\frac{1+z}{1-z}\tilde{f}$$

with $\tilde{g} \in L^2(\tilde{\mu})$. Let $\varphi = \tilde{U}\tilde{f} \in H$ and $\eta = \tilde{U}\tilde{g} \in H$. Since $i(1+z)\tilde{f} = (1-z)\tilde{g}$, then

$$i(1+V)\varphi = i\tilde{U}((1+z)\tilde{f}) = \tilde{U}((1-z)\tilde{g}) = (1-V)\eta.$$

We recall that

$$V = 1 - 2i(T+i)^{-1}$$

and hence

$$\varphi = \frac{1}{2}\big((1-V)\varphi + (1+V)\varphi\big) = i(T+i)^{-1}\varphi + (T+i)^{-1}\eta.$$

Thus $\varphi \in D(T)$ and

$$(T+i)\varphi = i\varphi + \eta$$

hence

$$T\varphi = \eta.$$

We may reverse the direction of the argument and obtain $\tilde{U} : D(M_\phi) \to D(T)$ via $\tilde{f} \to \varphi$ is bijective.

We define

$$\mu(I \times \{j\}) = \tilde{\mu}(\psi(I) \times \{j\}), \quad I \subset \mathbb{R},$$

with $\psi(x) = \frac{x-i}{x+i}$ such that $|\psi(x)| = 1$ and $\psi(x) \neq 1$ if $x \in \mathbb{R}$. This defines a unitary map $U^\sharp : L^2(\mu) \to L^2(\tilde{\mu})$ by

$$U^\sharp(f(x,j)) = \tilde{f}(z,j) := f(i\frac{1+z}{1-z}, j) \text{ with } z = \psi(x).$$

Hence $U^\sharp : D(M_x) \to D(M_\phi)$ is bijective and for any $f \in D(M_x)$

$$U^\sharp(M_x f) = i\frac{1+z}{1-z}f(i\frac{1+z}{1-z}, j) = M_\phi\tilde{f} = M_\phi U^\sharp f.$$

We define the unitary map $U = \tilde{U} \circ U^\sharp : L^2(\mu) \to H$ so that $U : D(M_x) \to D(T)$ is bijective and for any $f \in D(M_x)$

$$\begin{aligned} U(M_x f) = \tilde{U}(U^\sharp(M_x f)) &= \tilde{U}(M_\phi U^\sharp f) = \tilde{U}(M_\phi \tilde{f}) = \tilde{U}(\tilde{g}) = \eta \\ &= T\varphi = T\tilde{U}(\tilde{f}) = T\tilde{U}(U^\sharp f) = TUf. \end{aligned}$$

$\square$

3.7 Stone's theorem

Theorem 3.33 (Stone's theorem)**.** *Let T be a densely defined selfadjoint operator with domain $D(T)$. Then there is a unique strongly continuous unitary group $S(t)$ with $t \to S(t)\phi$ differentiable iff $\phi \in D(T)$ and*

$$\frac{d}{dt}S(t)\phi|_{t=0} = iT\phi.$$

This selfadjoint operator T is called the generator of the group $S(t) = e^{itT}$.

Let $S(t)$ be a unitary operator for every $t \in \mathbb{R}$ which satisfies

$$S(0) = 1, \quad S(s+t) = S(s)S(t)$$

and for all $\phi, \psi \in H$

$$t \to \langle S(t)\phi, \psi\rangle$$

is measurable. Then $S(t)$ is strongly continuous and there exists a unique generator of $S(t)$.

Proof. Let T be selfadjoint. By Theorem 3.32 it suffices to consider operators M_x densely defined on $L^2(\mu)$. e^{itx} is a unitary group on $L^2(\mu)$ and

$$t \to e^{itx}g$$

is differentiable with respect to t if $xg \in L^2(\mu)$, i.e. $g \in D(M_x)$:

$$\frac{e^{itx}-1}{t} \to ix \quad \text{as } t \to 0$$

and

$$\left|\frac{e^{itx}-1}{t}\right| \leqslant \frac{|tx|}{|t|} = |x|$$

and $t^{-1}(e^{itx}-1)g$ converges to ixg for $xg \in L^2(\mu)$ by the theorem of Lebesgue.

[24.05.2017]

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Let $S(t)$ be a unitary operator as in the theorem. For $f \in C_0^1(\mathbb{R})$ we define $A_f : H \mapsto H$ such that for any $\phi, \psi \in H$

$$\langle A_f\phi, \psi\rangle = \langle \int_{\mathbb{R}} f(t)S(t)\phi dt, \psi\rangle = \int_{\mathbb{R}} \langle f(t)S(t)\phi, \psi\rangle\, dt := \langle \int_{\mathbb{R}} f(t)S(t)dt\, \phi, \psi\rangle$$

where $\int_{\mathbb{R}} f(t)S(t)dt$ in the last equality is a tempting abuse of notation.

Let $A := A_{\chi_{t\geqslant 0}e^{-t}}$. Then noticing $S^*(t) = S(-t)$ we have

$$A^* = \int_{-\infty}^{0} e^t S(t)dt,$$

$$A + A^* = \int_{\mathbb{R}} e^{-|t|} S(t)dt$$

$$\begin{aligned} AA^* =& \int_0^\infty e^{-t} S(t)dt \int_{-\infty}^0 e^s S(s)ds \\ =& \int_0^\infty \int_0^\infty e^{-t-s} S(t-s)dtds \\ =& \int_{\mathbb{R}} \int_{0\leqslant s, \tau+s} e^{-\tau-2s} ds S(\tau)d\tau \\ =& \frac{1}{2}\int_{\mathbb{R}} e^{-|\tau|} S(\tau)d\tau = A^*A. \end{aligned}$$

We define $V = 1 - 2A$. Then $VV^* = V^*V = 1$. Consider

$$\begin{aligned} -\frac{2}{t}(S(t)-1)A =& \frac{2}{t}(A - S(t)A) \\ =& \frac{2}{t}\left(\int_0^\infty e^{-t}S(t)dt - \int_t^\infty e^{-s+t} S(s)ds\right) \\ =& 2e^t \frac{1}{t}\int_0^t e^{-s}S(s)ds - 2\frac{e^t-1}{t}\int_0^\infty e^{-s}S(s)ds \end{aligned}$$

hence

$$\lim_{t\to 0} \frac{S(t)-1}{t}(V-1)\phi \to (V+1)\phi$$

for all $\phi \in H$. $V\eta = \eta$ implies $0 = (V+1)\eta$ and hence also $\eta = 0$.

Using Theorem 3.23 we find a Radon measure on $\mathbb{S}^1 \times \mathbb{N}$ and a unitary map $U : L^2(\mu) \to H$ so that $Uzf = VUf$ and $U\bar{z}f = V^*Uf$. We define the selfadjoint multiplication operator by $i\frac{1+z}{1-z}$ with the domain $\{f \in L^2(\mu) : \frac{1}{1-z}f \in L^2(\mu)\}$. Let $\tilde{S}(t) = U^{-1}S(t)U : L^2(\mu) \mapsto L^2(\mu)$. Then

$$\lim_{t\to 0} \frac{\tilde{S}(t)-1}{t}(z-1)f \to (z+1)f$$

and in the domain we can devide by $z-1$ and obtain

$$\lim_{t\to 0} \frac{\tilde{S}(t)-1}{t}f \to -\frac{1+z}{1-z}f.$$

Then $M_{i\frac{1+z}{1-z}}$ is the generator of $\tilde{S}(t)$ and

$$T = UM_{i\frac{1+z}{1-z}}U^{-1}$$

is the generator of $S(t)$. $\square$

3.8 The Heisenberg group and quantization

3.8.1 The Heisenberg group

Recall that observables in quantum mechanics are selfadjoint operators. The most important operators are the position operators denoted by (X_j) $1 \leqslant j \leqslant d$ where X_j refers to the jth coordinate. The (e^{itX_j}) commute and generate a d dimensional group which we denote by

$$\mathbb{R}^d \ni \xi \to V(\xi) = e^{i\xi\cdot X}.$$

There is also a d dimensional translation group $U(y)$ which satisfies

$$U(y)XU(-y) = X + y$$

and, equivalently

$$U(y)e^{i\xi\cdot X}U(-y) = e^{i\xi\cdot y}e^{i\xi\cdot X}.$$

We may write these relations as

$$U(y)V(\xi) = e^{i\xi\cdot y}V(\xi)U(y), \tag{3.7}$$

which is called the Weyl form of the canonical commutation relations (CCR).

The simplest realization as a group of unitary operators on a Hilbert space is as follows: We take $H = L^2(\mathbb{R}^d)$. We define a strongly continuous homomorphism by

$$\begin{aligned} W(\xi, y, t)f(x) =& e^{it}e^{-i\frac{\xi\cdot y}{2}}e^{i\xi\cdot(x+y)}f(x+y) \\ =& e^{i(t-\frac{\xi\cdot y}{2})}U(y)V(\xi)f \\ =& e^{it}e^{i\frac{\xi\cdot y}{2}}e^{i\xi\cdot x}f(x+y) \\ =& e^{i(t+\frac{\xi\cdot y}{2})}V(\xi)U(y)f. \end{aligned}$$

Lemma 3.34. *We have*

$$W(\xi, x, t)W(\eta, y, s) = W(\xi + \eta, x + y, t + s + \frac{1}{2}(x\cdot\eta - y\cdot\xi)).$$

Proof.

$$\begin{aligned}W(\xi,x,t)W(\eta,y,s) =&e^{i(t+s)-\frac{i}{2}(\xi\cdot x+\eta\cdot y)}U(x)V(\xi)U(y)V(\eta)\\ =&e^{i(t+s-\frac{1}{2}\xi\cdot x-\frac{1}{2}y\cdot\eta-y\cdot\xi)}U(x)U(y)V(\xi)V(\eta)\\ =&e^{i(t+s+\frac{1}{2}(x\cdot\eta-y\cdot\xi)-\frac{1}{2}(x+y)\cdot(\xi+\eta))}U(x+y)V(\xi+\eta)\\ =&W(\xi+\eta,x+y,t+s+\frac{1}{2}(x\cdot\eta-y\cdot\xi)).\end{aligned}$$

□

One way to describe the structure is by a matrix group. Consider the matrices

$$A(x,\xi,t)=\begin{pmatrix}1 & x_1 & x_2 & \dots & x_d & t-\frac{1}{2}x\cdot\xi\\ 0 & 1 & 0 & \dots & 0 & \xi_1\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & 0 & \dots & 1 & \xi_d\\ 0 & 0 & 0 & \dots & 0 & 1\end{pmatrix}$$

where

$$A(x,\xi,t)A(y,\eta,s)=A\Big(x+y,\xi+\eta,s+t+\frac{1}{2}(x\cdot\eta-y\cdot\xi)\Big) \tag{3.8}$$

with

$$A(x,\xi,t)^{-1}=A(-x,-\xi,-t)$$

and identity $A(0,0,0)$. The matrix group is an affine subspace of the $(d+2)\times(d+2)$ matrices. It is called Heisenberg group H^d.

3.8.2 Quantization

Mathematical quantization provides a map from functions on $\mathbb{R}^{2d}$ to operators on function spaces on $\mathbb{R}^d$. This is related to quantization in physics, but we omit the Planck constant $\hbar$, which we define to be 1.

Let $a\in\mathcal{S}(\mathbb{R}^d\times\mathbb{R}^d)$. If $a(x,\xi)=e^{i(\eta\cdot x+y\cdot\xi)}$ then we want to have

$$W(a)=W(\eta,y,0)=e^{-i\frac{1}{2}\eta\cdot y}U(y)V(\eta)=e^{i\frac{1}{2}\eta\cdot y}V(\eta)U(y).$$

By the Fourier transform in both the two variables

$$\hat{a}(x,\xi)=\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d\times\mathbb{R}^d}a(\eta,y)e^{-i(\eta\cdot x+\xi\cdot y)}dyd\eta$$

and the Fourier inversion, we define

$$a^w(x,D)f(x) := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d\times\mathbb{R}^d}\hat{a}(\eta,y)W(\eta,y,0)f(x)dyd\eta, \tag{3.9}$$

which equals to

$$\begin{aligned}
&(2\pi)^{-d}\int_{\mathbb{R}^d\times\mathbb{R}^d}\hat{a}(\eta,y)e^{i(\eta\cdot x+\eta\cdot y/2)}f(x+y)dyd\eta\\
=&\frac{1}{(2\pi)^{2d}}\int_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}}a(\tilde{x},\xi)e^{i(-\tilde{x}\cdot\eta-y\cdot\xi+\eta\cdot x+\eta\cdot y/2)}f(x+y)d\tilde{x}d\xi dyd\eta\\
=&\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d\times\mathbb{R}^d}a(x+y/2,\xi)e^{-iy\cdot\xi}f(x+y)dyd\xi\\
=&\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d\times\mathbb{R}^d}a((x+y)/2,\xi)e^{i\xi\cdot(x-y)}f(y)dyd\xi,
\end{aligned}$$

where we used Fourier inversion for Schwartz functions $a(\cdot,\xi)$ as follows

$$(2\pi)^{-d}\int_{\mathbb{R}^d\times\mathbb{R}^d}g(\tilde{x})e^{i(x-y)\eta}d\tilde{x}d\eta = g(y).$$

$a^w(x,D)$ is called the Weyl quantization of a.

Lemma 3.35. *Suppose that* $a(x,\xi)\in\mathcal{S}(\mathbb{R}^d)$. *Then*

$$\|a^w(x,D)\|_{HS} = (2\pi)^{-\frac{d}{2}}\|a\|_{L^2(\mathbb{R}^{2d})}.$$

Moreover

$$a^w(x,D)b^w(x,D) = (a\sharp b)^w(x,D)$$

where

$$\mathcal{F}(a\sharp b)(\xi,x) = (2\pi)^{-d}\int_{\mathbb{R}^{2d}}e^{i\frac{1}{2}((x-y)\cdot\eta-y\cdot(\xi-\eta))}\hat{a}(\xi-\eta,x-y)\hat{b}(\eta,y)dyd\eta.$$

Proof. We calculate

$$\begin{aligned}
a^w(x,D)f(x) &= \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d\times\mathbb{R}^d}a((x+y)/2,\xi)e^{i\xi\cdot(x-y)}f(y)d\xi dy\\
&= \frac{1}{(2\pi)^{d/2}}\int_{\mathbb{R}^d}\mathcal{F}_2 a((x+y)/2,y-x)f(y)dy,
\end{aligned} \tag{3.10}$$

where $\mathcal{F}_2$ means the Fourier transform on the second variable, and

$$\|a\|_{L^2}^2 = \|\mathcal{F}_2 a\|_{L^2}^2 = \int_{\mathbb{R}^{2d}}|\check{\mathcal{F}}_2 a((x+y)/2,y-x)|^2dxdy.$$

This implies the first statement.

Then

$$a^w(x,D)b^w(x,D) = (2\pi)^{-2d} \int_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} \hat{a}(\xi,x)\hat{b}(\eta,y)W(\xi,x)W(\eta,y)dxd\xi dyd\eta$$

$$= (2\pi)^{-2d} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \hat{a}(\xi,x)\hat{b}(\eta,y)e^{i\frac{1}{2}(x\cdot\eta - y\cdot\xi)}W(\xi+\eta, x+y)dxd\xi dyd\eta$$

$$= (2\pi)^{-d} \int_{\mathbb{R}^{2d}} (2\pi)^{-d} \int_{\mathbb{R}^{2d}} \hat{a}(\xi-\eta, x-y)\hat{b}(\eta,y)e^{i\frac{1}{2}((x-y)\cdot\eta - y\cdot(\xi-\eta))}W(\xi,x)dxd\xi dyd\eta,$$

which implies the claimed formula. $\square$

[26.05.2017]

[31.05.2017]

3.9 The Theorem of Stone-von Neumann

Let $\mathbb{N}_N = \{1,\dots,N\}$ if $N < \infty$ and $\mathbb{N}$ if $N = \infty$. Let μ be the Radon measure on $\mathbb{R}\times\mathbb{N}_N$ which is the Lebesgue measure on $\mathbb{R}\times\{j\}$.

Theorem 3.36 (Stone-von Neumann). *Let H be a Hilbert space and $V(\xi)$ and $U(y)$, $\xi, y \in \mathbb{R}^d$ be strongly continuous unitary operators on H satisfying the Weyl commutation relations. Then there exist N and a unitary map*

$$R : L^2(\mathbb{R}^d \times \mathbb{N}_N)) \to H$$

so that $X : H \to H$ is unitarily equivalent to the multiplication by x,

$$R^{-1}XR = M_x$$

and

$$R^{-1}U(y)Rf = f(\cdot + y).$$

Proof. Step 1. **Claim**: There is no nontrivial closed invariant subspace for $L^2(\mathbb{R}^d)$. Indeed, suppose that there are $f, g \in \mathcal{S}(\mathbb{R}^d)$ such that

$$\langle W(\xi,y)f, g\rangle_{L^2(\mathbb{R}^d)} = 0 \tag{3.11}$$

for all $\xi, y \in \mathbb{R}^d$. Then

$$\langle a^w(x,D)f, g\rangle_{L^2(\mathbb{R}^d)} = 0$$

for all $a \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$.

Suppose that $\mathcal{F}_2 a((x+y)/2, y-x) = (2\pi)^{\frac{d}{2}} g(x)\overline{f(y)}$. This can be achieved by

$$\mathcal{F}_2 a(x,y) = (2\pi)^{\frac{d}{2}} g(x+y/2)\overline{f(x-y/2)}.$$

Then by (3.10) one has

$$a^w(x,D)f = \|f\|_{L^2}^2 g(x)$$

and (3.11) implies that $f=0$ or $g=0$. The claim follows by the density of $\mathcal{S}(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$.

Step 2. The function $e^{-|x|^2/2}$ is cyclic for the Cayley operators $\tilde{C}_j$ of M_{x_j} (which commute). To see this we observe that for every cube $I_1 \times \dots \times I_d$

$$\chi_{I_1\times \dots \times I_d} e^{-|x|^2/2}$$

is in the closure of the span of $\tilde{C}_{j_1} \cdots \tilde{C}_{j_k}$, since we may express them by multiplications by characteristic functions in the spectral representation of the $\tilde{C}_j$.

Step 3. Let

$$\mathcal{F}_2 a(x,y) = (2\pi)^{\frac{d}{2}} e^{-\frac{1}{2}|x-y/2|^2} e^{-\frac{1}{2}|x+y/2|^2}.$$

Then by view of (3.10)

$$a^w(x,D)f(x) = \int_{\mathbb{R}^d} e^{-\frac{1}{2}|y|^2} f(y)dy\, e^{-\frac{1}{2}|x|^2},$$

and hence $a^w(x,D)$ is a projector to the span of $e^{-\frac{1}{2}|x|^2}$. Thus $a\sharp a = a$ (see Lemma 3.35).

We now use $a^w(x,D)$ to define a projector on H by (3.9). Let Y be its range in H. It is closed since it is the null space of $1-a^w(x,D)$. We choose an ONB basis $\{\phi_j\}$ in Y and define H_j by the closure of the space of $W(\xi,y)\phi_j$.

By the Weyl commutation relations $V(te_k)$ commutes with $V(se_j)$. By the exercise also the Cayley transforms C_k and their adjoints C_k^* commute. Thus $\frac{1}{2}(C_k + C_k^*)$ and $\frac{1}{2i}(C_k - C_k^*)$ are commuting selfadjoint operators. Let $\tilde{H}_j$ be the span of $C_k^m \phi_j$ and $(C_k^m)^*\phi_j$. By Theorem 3.20 there exist a unique measure μ on $(S^1)^d$ and unique unitary maps $\tilde{R}_1 : L^2(\mu) \to \tilde{H}_j$ and $\tilde{R}_2 : L^2(\mu) \to L^2(\mathbb{R}^d)$ so that

$$\tilde{R}_1 1 = \phi_j, \quad \tilde{R}_2 1 = (2\pi)^{-\frac{d}{2}} e^{-\frac{|x|^2}{2}},$$

$$\tilde{R}_1(z^\alpha \bar{z}^\beta) = C^\alpha (C^\beta)^* \phi_j$$

$$\tilde{R}_2(z^\alpha \bar{z}^\beta) = \left(\frac{1+ix}{1-ix}\right)^\alpha \left(\frac{1-ix}{1+ix}\right)^\beta (2\pi)^{-\frac{d}{2}} e^{-\frac{|x|^2}{2}}.$$

We define $R_j = \tilde{R}_1(\tilde{R}_2)^{-1}$. Then

$$R_j x_j f = X_j R_j f$$

where X_j is the generator of $V(t\xi_j)$ and also

$$R_j e^{i\xi\cdot x} f = V(\xi) R_j f.$$

Step 4. Since

$$e^{-|x+y|^2/2} = e^{-x\cdot y - |y|^2/2} e^{-|x|^2/2}$$

we obtain

$$e^{-|x+y|^2/2} = (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} \mathcal{F}(e^{-x\cdot y-|y|^2/2})(\xi) W(\xi,0,0) d\xi \, e^{-|x|^2/2}$$

and hence with the projector $a^w(x,D)$ from above

$$\left[U(y) - (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} \mathcal{F}(e^{-x\cdot y-|y|^2/2})(\xi) W(\xi,0,0) d\xi \right] a^w(x,D) = 0.$$

As a consequence

$$\begin{aligned} U(y) R_j((2\pi)^{-\frac{d}{2}} e^{-|x|^2/2}) &= U(y)\phi_j \\ &= (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} \mathcal{F}(e^{-x\cdot y-|y|^2/2})(\xi) V(\xi) R_j((2\pi)^{-\frac{d}{2}} e^{-|x|^2/2}) d\xi \\ &= R_j (2\pi)^{-d} \int_{\mathbb{R}^d} \mathcal{F}(e^{-x\cdot y-|y|^2/2})(\xi) e^{i\xi\cdot x} e^{-|x|^2/2} d\xi = R_j (2\pi)^{-\frac{d}{2}} e^{-|x+y|^2/2}. \end{aligned}$$

We claim that the closure of the space of $e^{-|x+y|^2/2}$ is $L^2(\mathbb{R}^d)$. After a Fourier transform this is equivalent to the statement that the closure of span $e^{i\xi\cdot x} e^{-|x|^2/2}$ is $L^2(\mathbb{R}^d)$. In Step 2 we have seen that $e^{-|x|^2/2}$ is cyclic for the Cayley transforms and there adjoints. By the proof of Theorem 3.31 this implies that $e^{-|x|^2/2}$ is cyclic for $(x_j \pm i)^{-1}$. But this implies as in Step 3 that $L^2(\mu)$ is the closure of the span of $e^{i\xi\cdot x} e^{-|x|^2/2}$. Then

$$U(y) R_j f = R_j f(\cdot + y).$$

Step 5. To conclude we put all the unitary operators R_j together.

□

3.9.1 The uncertainty principle

It is an immediate consequence of the commutation relations that for $\phi \in \mathcal{S}(\mathbb{R}^d)$

$$0 = \frac{d}{ds}\frac{d}{dt}\big[\big(U(te_j)V(se_j) - e^{ist}V(se_j)U(te_j)\big)\phi\big]_{s=t=0} = (i\partial_j x_j - ix_j\partial_j - i)\phi$$

and hence

$$[i\partial_j, x_k] = i\delta_{jk}.$$

Theorem 3.37. *The following inequality always holds:*

$$2\|xf\|_{L^2(\mathbb{R}^d)}\|k\hat{f}\|_{L^2(\mathbb{R}^d)} \geqslant \|f\|^2_{L^2(\mathbb{R}^d)}.$$

Proof. We calculate for Schwartz functions and $d = 1$

$$\begin{aligned} \|f\|^2_{L^2} = \langle f, f\rangle = \langle [\partial, x]f, f\rangle &= \langle \partial(xf), f\rangle - \langle x\partial f, f\rangle \\ &= -\langle xf, \partial f\rangle - \langle \partial f, xf\rangle \leqslant 2\|xf\|_{L^2}\|\partial f\|_{L^2}. \end{aligned}$$

□

Remark 3.38. *We get an identity if $\partial f + xf = 0$ which is equivalent to $f = ce^{-\frac{|x|^2}{2}}$.*

4 Schrödinger operators with potentials

4.1 Hamiltonian mechanics and quantum mechanics

The first step in quantum mechanics is to formulate the quantization of Hamiltonian dynamics. Particularly relevant cases are particles in a potential field (protons and neutrons in a nucleus), charged particles in an electric or magnetic field (like electrons in an atom) and systems of many charged particles (heavy atoms).

The independent variables are the position x and the momentum p where for a particle of mass m, $p = mv$ where v is the velocity. The Hamilton function $H(x,p)$ is the energy of a system. The dynmacics are then described by teh Hamiltonian equations

$$\dot{x}_j = \frac{\partial H}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial H}{\partial x_j} \tag{4.1}$$

[31.05.2017]

[02.06.2017]

1. For a free particle the Hamiltonian is the kinetic energy $\frac{1}{2}m|v|^2 = \frac{1}{2m}|p|^2$. The dynamics is described by the Hamiltonian equations

$$\dot{x}_j = \partial_{p_j} H(p,x) \qquad \dot{p}_j = -\partial_{x_j} H(p,x).$$

For a free particle of mass m this gives

$$\dot{x}_j = \frac{1}{m} p_j, \quad \dot{p}_j = 0, \quad \ddot{x}_j = 0$$

and

$$x_j(t) = x_j(0) + \frac{1}{m} p_j(0) t, \qquad p_j(t) = p_j(0).$$

2. A particle trapped by a quadratic potential $\frac{1}{2}|x|^2$ is described by the Hamilton function

$$H(x,p) = \frac{1}{2m}|p|^2 + \frac{1}{2}|x|^2.$$

The Hamiltonian equations are

$$\dot{x}_j = \frac{1}{m} p_j, \qquad \dot{p}_j = -x_j$$

with the solution

$$x_j(t) = \cos(t/\sqrt{m}) x_j(0) + \frac{1}{\sqrt{m}} \sin(t/\sqrt{m}) p_j(0)$$

$$p_j(t) = -\sqrt{m} \sin(t/\sqrt{m}) x_j(0) + \cos(t/\sqrt{m}) p_j(0).$$

3. Two particles of mass m_1 and m_2 at position x and y feel the gravitational force

$$F(x,y) = G m_1 m_2 \frac{x-y}{|x-y|^3}$$

where

$$G \sim 6.67408(31) \times 10^{-11} m^3\, kg^{-1}\, s^{-2}.$$

Mass is measured in kg, time in seconds sec and length in meter m, velocity in m/s , acceleration in m/s^2 and force in Newton N

$$1N = 1kg\, m/sec^2.$$

The acceleration by the gravitational force of two particles of mass $1kg$ and distance $1m$ is

$$\sim 6.67408(31) \times 10^{-11} m\, s^{-2}.$$

The Hamiltonian for two particles in a gravitational field is

$$H(x, y, p_1, p_2) = \frac{1}{2m_1}|p_1|^2 + \frac{1}{2m_2}|p_2|^2 - \frac{Gm_1m_2}{|x-y|}$$

and the Hamiltonian equations are

$$\dot{x} = \frac{1}{m_1}p_1, \qquad \dot{y} = \frac{1}{m_2}p_2$$

$$\dot{p}_1 = \frac{Gm_1m_2}{|x-y|^3}(y-x) \quad \dot{p}_2 = \frac{Gm_1m_2}{|x-y|^3}(x-y).$$

For a system of n particles of mass m_j we obtain the Hamiltonian

$$H(x_j, p_j) = \sum_{j=1}^{n} \frac{1}{2m_j}|p_j|^2 - \sum_{j\neq k} \frac{Gm_jm_k}{|x_j - x_k|}.$$

The solutions to the two particle system are essentially described by Kepler's laws. The n particle system is relevant for the solar system.

4. The electrostatic potential is similar to the gravitational potential, but now with charges replacing mass, and charges may have both signs: Equal charges repel and different charges attract. The electrostatic potential is much stronger than the gravitational potential, but matter tends to be neutral on moderate scales. If q_1 and q_2 are the electric charges then the force is

$$F = \frac{1}{4\pi\epsilon_0}\frac{q_1q_2}{|x-y|^3}(x-y).$$

Charges are measured in Coulomb C and the vacuum permittivity ϵ_0 is given by

$$\epsilon_0 = \frac{10^{-9}}{36\pi}C^2N^{-1}m^{-2}.$$

A natural unit is to measure charge in multiples of the charge of an electron. Coulomb is often more handy. The charge of an electron is about $1.60210^{-9}C$.

5. Charged particles generate an electric field $E : \mathbb{R}^d \to \mathbb{R}^d$, and they feel an electric field. It is measured in newton per coulomb. The Hamiltonian for a charged particle with charge q in an electric field with potential U (i.e. $E = -\nabla U$) is

$$H(x, p) = \frac{1}{2m}|p|^2 + qU(x)$$

The Hamiltonian equations are derived as above.

6. $d = 3$ Moving charged particles generate a magnetic field, and they feel a magnetic field $B : \mathbb{R}^3 \to \mathbb{R}^3$. Consider a fixed magnetic field. A charged particle feels a force, which is proportional to the charge, the velocity, and strength of the field, and which is perpendicular to both the field and the velocity. As a consequence a charged particle moves along spirals in a constant magnetic field. The charged particle feels the force
$$q(E + \frac{p}{m} \times B)$$
where E is the electric field and B is the magnetic field. Consider a constant magnetic field B. There is no source and one always has
$$\nabla \cdot B = 0$$
and there is a vector potential A for a magnetic field defined on $\mathbb{R}^3$,
$$B = \nabla \times A.$$
The Hamiltonian of a single charged particle is
$$H(x,p) = \frac{1}{2m}|p - qA|^2 + qV.$$

Properties of Hamiltonian dynamics:

1. The Hamiltonian equations are a system of ordinary differential equations. Standard theory gives local existence of solutions.

2. The Hamiltonian is preserved and has an interpretation as energy.

3. The evolution is called Hamiltonian flow. It preserves the symplectic structure of $\mathbb{R}^d$.

4.1.1 Quantization

In quantum physics the time evolution is a unitary evolution, and, if the system does not depend on time explictly, it is a unitary evolution.

The basic rule of quantum mechanics is that we quantize a classical system with Hamiltonian H by setting $a(x,p) = H(x, \hbar p)$, and define the Hamilton operator (again denoted by H, here $\tilde{H}$)
$$\tilde{H} = a^w(x, D)$$
and reparametrize time by $\frac{1}{\hbar}t$. We obtain
$$i\hbar\partial_t\Psi + \frac{\hbar^2}{2m}\Delta\Psi = 0$$

for the free particle and

$$i\hbar\partial_t\Psi + \frac{\hbar^2}{2m}\Delta\Psi - \frac{1}{2}|x|^2\Psi = 0$$

for the quantum harmonic oscillator.

4.1.2 Units and scales

The SI (frz. Système international d'unités) base units are g, meter m, second s, Newton N (force), and the current measure in Ampere A and energy in Joule J.

Planck's constant is

$$\hbar = 6.62607004 \times 10^{-34} m^2 kg/s.$$

The Planck length is

$$l_P = \sqrt{\frac{\hbar G}{c^3}} \sim 1.616229 \times 10^{-35} m$$

where G is the gravitation constant and c is the speed of light. Similarly one may define the Planck time and a Planck mass. These are absolute units, but they are very small.

What are the scales of the objects of interest? The mass of an electron is around

$$m_e \sim 9.10938356 \times 10^{-31} kg$$

and the mass of the neutron is around

$$m_n = 1.675 \times 10^{-27} kg$$

and the proton mass is around

$$m_p = 1.676219 \times 10^{-27} kg.$$

The radius of a nucleus is approximately $R = 1.25 \times 10^{-15} m A^{\frac{1}{3}}$ where A is the number of protons and neutrons.

The Bohr radius of hydrogen is $\sim 0.529177 \times 10^{-10}$m. The nucleus of an atom contains most of the mass, and a tiny but of the volume. It is a reasonable approximation to consider a coordinate system so that the nucleus is at the position $x = 0$. Its charge q is a multiple n of the charge of an electron q_e, and the most reasonable system is the one of m electrons. We obtain the Hamiltonian (neglecting magnetic fields)

$$H(x_j, p_j) = \frac{1}{m_e} \sum_{j=1}^{n} \left(|p_j|^2 - n q_e^2 \frac{1}{|x_j|} \right) + \sum_{j \neq k} q_e^2 \frac{1}{|x_j - x_k|}. \tag{4.2}$$

A useful unit is the electron volt: $1\text{eV} = 1.6021766208 \times 10^{-19}$ Joule.

Quantum mechanics is most relevant on the scale of atoms, in particular for the dynamics of the nucleus and the electron. The main force is the quantized electric (and magnetic) interaction.

The structure of the nucleus is determined by the strong force. In a certain regime it can be approximated by an harmonic oscillator. Weak interaction is responsible for decay of particles (mean lifetime of neutron: 881.5 s, decay into electron and proton).

[02.06.2017]

[14.06.2017]

4.1.3 The Copenhagen interpretation

(Bohr, Heisenberg 1925-1927)

1. Since the evolution is unitary we may restrict ourselves to the evolution of funtions of norm 1. This represents the state of a system.

2. A measurement corresponds to a selfadjoint operator A, and physically, to an interaction with a laboratory device. This interaction is not described by quantum mechanics.

3. The relevant quantity is

$$\langle A\psi(t), \psi(t)\rangle.$$

   It gives the expected value of the outcome of an experiment.

4. The measurement changes the state. The wave function collapses. In the simplest case A is a selfadjoint projection. In that case

$$\langle A\psi, \psi\rangle$$

   gives the probability that the state is the state represented by the projection. The measurement has a 0/1 outcome (1 means the state is in the range of the projection, 0 means $A\psi = 0$) , and the wave function is projected by A if the outcome of outcome is 1, and by $1 - A$ if the outcome is 0.

In the double slit experiment the measurement could be: The particle goes througth the upper slit. The measurement removes the interference from the observation.

We observe that

$$\|x_j\psi\|^2 = \int x_j^2|\psi|^2 dx$$

and

$$\|\partial_j\psi\|^2 = \langle -\partial_j^2\psi, \psi\rangle.$$

The uncertainty relation says that the product of the expected values is at least 1 - i.e. if I do many independent measurements of the square of the position and the square of the momentum then the product of the means is at least 1 (with $\hbar = 1$).

Unless we specifically consider physical quantities we will set $\hbar = 1$.

4.2 The free particle

The Fourier transform transforms the negative of the Laplace operator $-\Delta$ into the multiplication by $|k|^2$. This is a self-adjoint operator by Lemma 3.25. Its spectrum is $[0,\infty)$, which is immediate from the multiplication property. On the Fourier side the multiplier

$$(|\xi|^2 - z^2)^{-1}$$

is bounded on $\mathbb{R}^d$ for $\operatorname{Im} z > 0$ and defines an operator in $L^2(\mathbb{R}^d)$. For $d = 1$ and $d = 3$ you have calculated the fundamental solution, which is the inverse Fourier transform, for $z = i$. The same calculation works for other z as well. In $d = 1$ we obtain

$$g(x) = -\frac{1}{2iz}e^{iz|x|} \tag{4.3}$$

since

$$g' = -\frac{1}{2}\frac{x}{|x|}e^{iz|x|}$$

and

$$-g'' = \frac{iz}{2}e^{iz|x|} + \delta_0$$

and hence

$$-g'' - z^2 g = \delta_0.$$

For $d = 3$ it is

$$g(x) = -\frac{1}{4\pi iz|x|}e^{iz|x|}. \tag{4.4}$$

Again one computes

$$-\Delta g = z^2 g + \delta_0$$

as in the exercise.

Lemma 4.1. *The operator $-\Delta$ is selfadjoint with*

$$D(-\Delta) = H^2(\mathbb{R}^d) = \{f \in L^2(\mathbb{R}^d) : \partial_{jl}^2 f, \partial_j f \in L^2(\mathbb{R}^d), \quad 1 \leqslant j, l \leqslant d\}.$$

Its spectrum is $[0, \infty)$.

Proof. After a Fourier transform we want to determine the domain of the multiplication by $|k|^2$. It is $\{\hat{f} \in L^2(\mathbb{R}^d) : |k|^2\hat{f} \in L^2(\mathbb{R}^d)\}$. Then

$$\mathcal{F}(-i\partial_j f) = k_j \hat{f}$$

and

$$\begin{aligned}
\|\partial_j f\|_{L^2} &= \|k_j \hat{f}\|_{L^2(\mathbb{R}^d)} \leqslant \frac{1}{2}\|(1+|k|^2)\hat{f}\|_{L^2} \leqslant \frac{1}{2}(\|f\|_{L^2} + \|\Delta f\|_{L^2}),\\
\|\partial_{jl}^2 f\|_{L^2} &= \|k_j k_l \hat{f}\|_{L^2} \leqslant \frac{1}{2}\||k|^2\hat{f}\|_{L^2(\mathbb{R}^d)} = \frac{1}{2}\|\Delta f\|_{L^2}.
\end{aligned}$$

The spectrum of the multiplication by $|k|^2$ is $[0, \infty)$, and hence the same is true for $-\Delta$. □

The Schrödinger equation for a free particle is

$$i\partial_t \psi + \Delta\psi = 0$$

which transforms into

$$i\partial_t \hat{\psi} - |k|^2\hat{\psi} = 0.$$

This equation can easily be solved:

$$\hat{\psi}(t,k) = e^{-it|k|^2}\hat{\psi}(0,k) = \lim_{\varepsilon\to 0} e^{-(\varepsilon+it)|k|^2}\hat{\psi}(0,k).$$

The inverse Fourier transform of $e^{-(\varepsilon+it)|k|^2}$ is (Exercise Sheet 1, Nr2 and Nr 3),

$$\sqrt{4\pi(\varepsilon+it)}^{-d} e^{-\frac{|x|^2}{4(\varepsilon+it)}}$$

and hence

$$\psi(t,x) = (\sqrt{4\pi i t})^{-d} \int e^{i\frac{|x-y|^2}{4t}}\psi(0,y)dy. \tag{4.5}$$

Lemma 4.2. *The selfadjoint operator $-\Delta$ generates a unitary group $S(t) = e^{-it\Delta}$ on $L^2(\mathbb{R}^d)$. It satisfies*

$$\|S(t)f\|_{L^2(\mathbb{R}^d)} = \|f\|_{L^2(\mathbb{R}^d)}$$

$$\|S(t)f\|_{L^\infty(\mathbb{R}^d)} \leqslant (4\pi|t|)^{-\frac{d}{2}}\|f\|_{L^1(\mathbb{R}^d)}.$$

Proof. The $L^2 \to L^2$ estimate is equivalent to the unitarity of the group. The $L^1 \to L^\infty$ estimate for Schwartz functions follows immediately from (4.5). Schwartz functions are dense in $L^1(\mathbb{R}^d)$ and we obtain the estimate for all functions in L^1. □

The $L^1 \to L^\infty$ shows that solutions with initial data in L^1 decay. The solution ψ disperses then in the sense that it converges pointwise uniformly to 0, despite the invertibility of $S(t)$.

[14.06.2017]

[16.06.2017]

4.3 The harmonic oscillator

Here we consider quantization of the Hamilton function $H(x,p) = \frac{1}{2}|p|^2 + \frac{1}{2}|x|^2$ with $\hbar = 1$. The operator is $T = -\Delta + |x|^2$ with $D(T) = \{f \in H^2 : |x|^2 f \in L^2\}$. Obviously T is symmetric. For any multiindex we define

$$h_\alpha = (\partial - x)^\alpha e^{-|x|^2/2}.$$

We recall that

$$T = -\sum_{j=1}^d (\partial_{x_j} - x_j)(\partial_{x_j} + x_j) + d.$$

Then

$$\langle T\psi, \psi\rangle = \sum_{j=1}^d \|(\partial_{x_j} + x_j)\psi\|^2 + d\|\psi\|_{L^2}^2$$

$$Te^{-|x|^2/2} = de^{-|x|^2/2}$$

and

$$\begin{aligned} Th_\alpha =& T(\partial - x)^\alpha e^{-|x|^2/2} \\ =& \sum_{j=1}^d (-\partial_j + x_j)(\partial_j + x_j)(\partial - x)^\alpha e^{-|x|^2/2} \\ =& 2|\alpha|(\partial - x)^\alpha e^{-|x|^2/2} + (\partial - x)^\alpha T e^{-|x|^2/2} \\ =& (2|\alpha| + d)(\partial - x)^\alpha e^{-|x|^2/2}. \end{aligned}$$

The Hermite functions h_α are eigenfunctions of T with the eigenvalue $2|\alpha|+d$. They satisfy

$$\int h_\alpha h_\beta dx = 0 \qquad (4.6)$$

if $\alpha \neq \beta$ since

$$\int (\partial_j - x_j)e^{-|x|^2/2}(\partial_k - x_k)e^{-|x|^2/2}dx$$
$$= (-1)\int e^{-|x|^2/2}(\partial_k + x_k)(\partial_j - x_j)e^{-|x|^2/2}dx$$
$$= \begin{cases} 0 & \text{if } k \neq j, \\ 2\|e^{-|x|^2/2}\|_{L^2}^2 & \text{if } k = j, \end{cases}$$

where we have commuted the operators $(\partial_k + x_k)$ to the right. If we do this for every direction we obtain

$$\|h_\alpha\|_{L^2}^2 = 2^{|\alpha|}\alpha!\pi^{\frac{d}{2}}.$$

We have seen that T^{-1} is a compact operator (Exercise 4 on Sheet 3). It maps L^2 to $D(T)$ (again Exercise 4 on Sheet 3). Thus it has an ONB of eigenfunctions. Above we determined all eigenfunctions. In particular the normalized Hermite functions are a complete set of eigenfunctions and we can define an inverse of T by

$$T^{-1}h_\alpha = (2|\alpha| + d)^{-1}h_\alpha.$$

The definition of the unitary group is now explicit and easy:

$$U(t)h_\alpha = e^{it(2|\alpha|+d)}h_\alpha. \tag{4.7}$$

We collect the results.

Theorem 4.3. *The operator $T = -\Delta + |x|^2$ with domain $D(T) = \{f \in L^2 : |x|^2 f, \partial_{ij}^2 f \in L^2\}$ is selfadjoint. It defines a unitary group described by (4.7). The spectrum of T is $2\mathbb{N}_0 + d$. The normalized Hermite functions $(2^{|\alpha|}\alpha!\pi^{d/2})^{-1/2}h_\alpha$ are an orthonormal basis.*

4.4 Harmonic polynomials and spherical harmonics

Schrödinger operators with radial potentials are an important special class. We will diagonalize the angular part of the operator using spherical harmonics.

Lemma 4.4. *The dimension of the space of homogeneous polynomials in $\mathbb{R}^d$ of degree m is $\binom{d+m-1}{d-1}$.*

Proof. The monomials of degree m are a basis of the homogeneous polynomials of degree m. The dimension is the set of all multiindices of length m. This is the number of possibilities of putting m objects into d boxes. Equivalently we may count the possibilities to put $d-1$ bars between m objects, or choosing $d-1$ out of $m+d-1$ objects. $\square$

Definition 4.5. *A spherical harmonic is a homogeneous harmonic polynomial.*

We recall the Euler identity for homogeneous functions of degree d:

$$x \cdot \nabla f = df.$$

Lemma 4.6. *Let f be a spherical harmonic of degree m. Then*

$$-|x|^2 \Delta f(x/|x|) = m(m-2+d) f(x/|x|).$$

Proof. We have (noticing that $\sum_{j=1}^d x_j \partial_j (f(x/|x|)) = 0$)

$$\begin{aligned} 0 =& \Delta f \\ =& \Delta(|x|^m f(x/|x|)) \\ =& |x|^m \Delta f(x/|x|) + m \nabla \cdot (|x|^{m-2} x) f(x/|x|) \\ =& |x|^{m-2} \Big(|x|^2 \Delta f(x/|x|) + m(m-2+d) f(x/|x|) \Big). \end{aligned}$$

$\square$

Lemma 4.7. *Let g and h be real homogeneous harmonic polynomials of degree $d_g \neq d_h$. Then g and h are orthogonal in the following sense*

$$\int_{\mathbb{S}^{d-1}} gh d\mathcal{H}^{d-1} = 0.$$

Proof. By the Euler identity and the divergence theorem

$$\begin{aligned} d_g \int_{\mathbb{S}^{d-1}} gh d\mathcal{H}^{d-1} =& \int_{\mathbb{S}^{d-1}} (x \cdot \nabla g) h d\mathcal{H}^{d-1} \\ =& \int_{B_1(0)} \nabla \cdot (\nabla g h) dx \\ =& \int_{B_1(0)} \nabla \cdot (g \nabla h) dx \\ =& \int_{\mathbb{S}^{d-1}} g x \cdot \nabla h d\mathcal{H}^{d-1} \\ =& d_f \int_{\mathbb{S}^{d-1}} gh d\mathcal{H}^{d-1} \end{aligned}$$

which implies the claim. $\square$

Definition 4.8. *We denote the space of homogeneous harmonic polynomials of degree N by V_N.*

Lemma 4.9. *Let p be a homogeneous polynomial of degree m. Then*

$$\Delta(|x|^{2-d-2m}p) = |x|^{2-d-2m}\Delta p.$$

Proof. Let $t \in \mathbb{R}$. We have

$$\begin{aligned}\Delta(|x|^t p) =&|x|^t\Delta p + 2t|x|^{t-2}x\cdot\nabla p + t(t+d-2)|x|^{t-2}p\\ =&|x|^t\Delta p + t(2m+t+d-2)|x|^{t-2}p\end{aligned}$$

where we used Euler's formula for the last equality. Set $t = 2-d-2m$. □

Lemma 4.10. *Let p be homogeneous of degree m and $d \geqslant 3$. Then*

$$p(\partial)|x|^{2-d} = |x|^{2-d-2m}\Big(\prod_{j=0}^{m-1}(2-d-2j)p(x) + |x|^2 q\Big)$$

where q is homogeneous of degree $d-2$. The left hand side is harmonic for $x \neq 0$.

Proof. The left hand side is the derivative of the fundamental solution. Hence it is harmonic away from the origin. It suffices to verify the identity for monomials. We prove it by induction on m. Suppose for $|\alpha| = m$

$$\partial^\alpha|x|^{2-d} = |x|^{2-d-2m}\Big(\prod_{j=0}^{m-1}(2-d-2j)x^\alpha + |x|^2 q_0\Big)$$

where q_0 has degree $m-2$. Then

$$\partial_{x_j}\partial^\alpha|x|^{2-d} = |x|^{2-d-2(m+1)}\Big(\prod_{j=0}^{m}(2-d-2j)x_j x^\alpha + |x|^2 r\Big)$$

with

$$r = (2-d-2m)x_j q_0 + \partial_j\Big(\prod_{j=0}^{m-1}(2-d-2j)x^\alpha + |x|^2 q_0\Big).$$

□

We obtain as immediate consequence

Lemma 4.11. *If p is a homogeneous polynomial of degree m then*

$$p(x) = \frac{1}{c_m}\Big(|x|^{d-2+2m}p(\partial)|x|^{2-d} + |x|^2 q\Big)$$

with $c_m = \prod_{j=0}^{m-1}(2-d-2j)$, for some homogeneous polynomial q of degree $m-2$.

Lemma 4.12. *Let f be a homogeneous polynomial of degree m. Then there exist unique harmonic polynomials p_j of degree j with $m-j \in 2\mathbb{Z}$ so that*

$$f = \sum_{j=0}^{[d/2]} |x|^{2j} p_{m-2j}$$

where

$$p_m = \frac{1}{c_m}|x|^{d-2+2m}p(\partial)|x|^{2-d}.$$

Proof. By lemma 4.11 and induction any homogeneous polynomial of degree m can be written as a sum

$$p = \sum_{j=0}^{[m/2]} |x|^{2j} h_{m-2j}$$

where h_{m-2j} is a harmonic polynomial of degree $m-2j$. To prove uniqueness suppose that we have two harmonic polynomials which agree on the unit ball. Then the difference vanishes by the maximum principle for harmonic functions. The formula is now a consequence of the second part of Lemma 4.11. $\square$

Let $a_m = \dim V_m$. By Lemma 4.4 and Lemma 4.12

$$\binom{d+m-1}{d-1} = \sum_{j=0}^{[m/2]} \dim V_{m-2j}$$

and hence

Lemma 4.13.

$$\dim V_m = \binom{d+m-1}{d-1} - \binom{d+m-3}{d-1}.$$

In particular, if $d=2$ then $\dim V_m = 2$ and V_N has the basis $\operatorname{Re}(x_1+ix_2)^m$ and $\operatorname{Im}(x_1+ix_2)^m$. If $d=3$ then

$$\dim V_m = 2m+1.$$

Let $f \in C^2(\mathbb{S}^{d-1})$. We define the Laplace-Beltrami operator on the sphere by

$$\Delta_{\mathbb{S}^{d-1}} f = \Delta f(x/|x|)\big|_{|x|=1}.$$

Theorem 4.14. *The operator $-\Delta_{\mathbb{S}^{d-1}}$ is selfadjoint with the domain*

$$D(-\Delta_{\mathbb{S}^{d-1}}) = \{f \in L^2(\mathbb{S}^{d-1}) : f(x/|x|) \in H^2(B_2(0)\backslash B_{\frac{1}{2}}(0))\}.$$

It has the eigenvalues $\{m(m+d-2) : m \in \mathbb{N} \cup \{0\}\}$ with eigenspace V_m. The span of $\{V_m\}$ is dense in $L^2(\mathbb{S}^{d-1})$.

Proof. Step 1: $-\Delta_{\mathbb{S}^{d-1}}$ maps $\{f \in L^2(\mathbb{S}^{d-1}) : f(x/|x|) \in H^2(B_2(0)\backslash B_{\frac{1}{2}}(0))\}$ to $L^2(\mathbb{S}^{d-1})$. This is immediate since

$$-|x|^2 \Delta f(x/|x|) = (\Delta_{\mathbb{S}^{d-1}} f)(x/|x|).$$

Step 2: Elliptic regularity gives

$$\sum_{j,k=1}^{d} \|\partial^2_{jk} u\|_{L^2(B_2(0)\backslash B_{\frac{1}{2}}(0))} \leqslant c\Big(\|\Delta u\|_{L^2(B_3(0)\backslash B_{\frac{1}{3}}(0))} + \|u\|_{L^2(B_3(0)\backslash B_{\frac{1}{3}}(0))}\Big).$$

This immediately implies the closedness of $-\Delta_{\mathbb{S}^{d-1}}$ with the given domain.

By the theorem of Stone-Weierstraß we can approximate every continuous function on $\mathbb{S}^{d-1}$ by a polynomial. By Lemma 4.12 we can approximate it by a sum of harmonic polynomials. By Lemma 4.6 homogeneous harmonic polynomials are eigenfunctions with the eigenvalues in the set of the theorem. Thus the list of eigenvalues is complete. It is now easy to see selfadjointness and positive semidefiniteness by decomposing polynomials into sums of homogeneous harmonic polynomials. □

4.5 The Coulomb potential 1: The discrete spectrum

The Schrödinger equation of a charged particle in a stationary electric field of a point mass is

$$i\hbar \frac{d}{dt}\psi + \frac{\hbar^2}{2m_e}\Delta\psi + \frac{Ze^2}{r}\psi = 0.$$

We restrict our consideration to the relevant case $d = 3$. Here e is the charge of the electron in *unrationalized electrostatic* units for which $e^2/\hbar c \sim \frac{1}{137}$ and

Z is the number of protons. We will see later that this equation defines a unitary evolution, or equivalently, that

$$\psi \to -\frac{\hbar^2}{2m_e}\Delta\psi - \frac{Ze^2}{r}\psi$$

defines a selfadjoint operator on a suitable domain D. We will see that the spectrum consists of the union $[0, \infty)$ and a countable sequence of negative eigenvalues accumulating at 0. The continuous spectrum $[0, \infty)$ corresponds to scattering states and the eigenvalues to bound states. This Schrödinger operator is a building block for quantum chemistry and the spectral lines of atoms. It provides a link between fundamental properties of atoms and observations. The picture is however incomplete and we will study the essential impact of symmetries and spin and scattering lateron.

In this subsection we will study the eigenvalues. We consider

$$-\frac{\hbar^2}{2m_e}\Delta\psi - \frac{Ze^2}{r}\psi = E\psi$$

where $E = -\frac{\hbar^2\kappa^2}{2m_e}$, $\kappa > 0$ is the energy.

We search for solutions in L^2, and, more precisely, of the form

$$\psi(x) = \frac{\kappa}{|x|}u(|x|/\kappa)h(x/|x|) \tag{4.8}$$

where h is a harmonic polynomial of degree l. This is a solution provided

$$-\frac{d^2}{dr^2}u + \Big[-\frac{\xi}{r} + \frac{l(l+1)}{r^2}\Big]u = -u$$

where

$$\xi = \frac{2m_eZe^2}{\kappa\hbar^2}.$$

We search for solutions $|u| \leqslant r^{l+1}$ as $r \to 0$ and approximately e^{-r} as $r \to \infty$ so we write

$$u = r^{l+1}e^{-r}F(r).$$

Since

$$\frac{du}{dr} = r^{l+1}e^{-r}\Big[\Big(\frac{l+1}{r} - 1\Big)F + \frac{dF}{dr}\Big]$$

and

$$\frac{d^2u}{dr^2} = r^{l+1}e^{-r}\Big[\Big(1 - \frac{2(l+1)}{r} + \frac{l(l+1)}{r^2}\Big)F + \Big(-2 + \frac{2(l+1)}{r}\Big)\frac{dF}{dr} + \frac{d^2F}{dr^2}\Big],$$

we obtain
$$\frac{d^2F}{dr^2} - 2\Big(1 - \frac{l+1}{r}\Big)\frac{dF}{dr} + \Big(\frac{\xi - 2l - 2}{r}\Big)F = 0. \tag{4.9}$$
This is a special hypergeometric differential equation and should be considered as a differential equation for which almost every information is explicitly available. We search for power series solutions

$$F = \sum_{j=0}^{\infty} a_j r^j$$

and we obtain

$$\begin{aligned} 0 &= \sum_{j=0}^{\infty} a_j \Big(j(j-1)r^{j-2} - 2jr^{j-1} + 2j(l+1)r^{j-2} + (\xi - 2l - 2)r^{j-1}\Big) \\ &= \sum_{j=0}^{\infty} r^{j-1}\Big[j(j+1)a_{j+1} - 2ja_j + 2(j+1)(l+1)a_{j+1} + (\xi - 2l - 2)a_j\Big]. \end{aligned}$$

This allows to compute a_j recursively from a_0:

$$(j + 2l + 2)(j+1)a_{j+1} = (-\xi + 2j + 2l + 2)a_j.$$

For large j
$$|a_{j+1}/a_j| \to 2/j$$
and
$$a_j \sim \prod_{k<j} 2/k \sim C2^j/\Gamma(1 + j + B).$$
Hence
$$F(r) \sim C\sum_{j=0}^{\infty} \frac{(2r)^j}{\Gamma(j+B+1)} \to C(2r)^{-B}e^{2r}$$
and
$$\psi \sim e^{|x|/\kappa}$$
for r large. This is in conflict with $\psi \in L^2(\mathbb{R}^3)$ unless the power series terminates, which happens iff $\xi = 2n$ for some positive integer $n > l + 1$. In this case the power series terminates with a multiple of r^{n-l-1}. The polynomials $F(r)$ are called Laguerre polynomials and written as $L^{2l+1}_{n-l-1}(2r)$ with the Rodriguez formula (without proof)

$$L^k_n(x) := \frac{e^x x^{-k}}{n!}\frac{d^n}{dx^n}(x^{n+k}e^{-x}).$$

They are orthogonal for the measure $\chi_{[0,\infty)}x^k e^{-x}dx$. We obtain

$$F = 1 \quad \text{if } n = l+1, \qquad F = 1 - \frac{r}{l+1} \text{ if } n = l+2.$$

It is remarkable that the enery only depends on n and not on l! We obtain

$$\kappa_n = \frac{2m_e Ze^2}{\xi\hbar^2} = \frac{1}{na}$$

where a is the Bohr radius

$$a = \frac{\hbar^2}{m_e Ze^2} = 0.5219177249 \times 10^{-8} Z^{-1} cm.$$

This is motivated since κ^{-1} is the decay rate for ψ given by the exponential in (4.8). The wave function ψ is well localized in $B_{na}(0)$. We obtain the bound state energies

$$E_n = -\frac{\hbar^2\kappa_n^2}{2m_e} = -\frac{13.605698Z^2eV}{n^2}$$

for the single electron hydrogen ($Z = 1$) and the partially ionized Helium ($Z = 2$).

The difference between the two lowest eigenvalues for hydrogen is around $10.2eV$. For each n we have l between 0 and $n-1$, and for each l there is a $2l+1$ dimensional space of harmonic polynomials of degree l. So the total number of states (dimension) with energy E_n is n^2. There is a standard nomeclature in chemestry for these states/eigenfunctions. The states with $l = 0$ are labelled by s *sharp* , the ones with $l = 1$ by p *principal* , the ones by $l = 2$ by d *diffuse* and the ones with $l = 3$ by f. The lowest state is labelled by $1s$, next $2s$, $2p$, $3s$, $3p$ and $3d$.

Atoms react with light by moving an electron to a different state, thereby emitting or absorbing a photon which carries the difference in energy,

$$E = 2\pi\hbar\nu$$

where ν is after de-Broglie the frequency which corresponds to light at a wavelength

$$\lambda = c/\nu.$$

For the transition from $1s$ to $2s$ the wave length is

$$\lambda \sim 10^{-6}m.$$

4.6 Complex differential equations and the hypergeometric equation

This is a short survey on the hypergeometric ODE. We consider a m order complex differential equation in the complex plane

$$u^{(m)} = F(z, u, u', \dots, u^{(m-1)})$$

with initial data

$$u^{(j)}(z_0) = u^j$$

where F is holomorphic in a neighborhood of the initial data.

Theorem 4.15. *There exists a unique holomorphic solution in a neighborhood of z_0.*

Proof. We provide only a sketch of the proof. Along lines we obtain an ODE which has a unique solution. This gives a candidate for a solution in a neighborhood, but one has to verify that u defined in this fashion satisfies the Cauchy-Riemann differential equations. Thus is done similarly as in the construction of potentials for vector fields F which satisfy

$$\frac{\partial F_j}{\partial x_l} = \frac{\partial F_l}{\partial x_j}.$$

□

Linear equations are a particular case. The equation

$$u' = au \tag{4.10}$$

has the exponential e^{az} as solution. Another one is the equation

$$zu' = au$$

where $a \in \mathbb{C}$. Remove the ray $(-\infty, 0]$ and write $z = \exp(y)$ with $|\operatorname{Im} y| < \pi$. Then the equation is equivalent to

$$\frac{du}{dy} = au,$$

$$u(y) = Ce^{ay} = Ce^{a \ln z} = Cz^a.$$

We can easily replace u by a vector U and a by a matrix A. A point of this type is called regular singular. The eigenvalues of A are the characteristic exponents.

Equations on $\mathbb{C}$ and more precisely the Riemann sphere are of particular interest.

The solutions to

$$(z-b)u' = au \tag{4.11}$$

are $(z-b)^a$ where we have to choose a branch of the logarithm.

[21.06.2016]

[23.06.2017]

We turn to second order equations

$$u'' = g(z)u' + h(z)u$$

with rational functions g and h.

The Riemann sphere $\bar{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$ is equipped with the coordinate maps

$$z : \bar{\mathbb{C}}\backslash\{\infty\} = \mathbb{C} \to \mathbb{C}, \quad z^{-1} : \bar{\mathbb{C}}\backslash\{0\} \to \mathbb{C}.$$

Then there are a finite number of poles of the coefficients g and h on the Riemann sphere.

A fact: Given a three tuple of pairwise disjoint points z_0, z_1, z_2 on the Riemann sphere there is a Möbius transform (biholomorphic map of the form

$$z \to \frac{a_1 z + b_1}{c_1 z + d_1}$$

with $a_1 d_1 - b_1 c_1 = 0$) which maps $(0, 1, \infty)$ to these three points.

We call a singular point z_0 *regular* if the equation can be written as first order system of the form

$$(z - z_0)\frac{dU}{dz} = f(z)U$$

with f holomorphic near z_0 and matrix valued. $z_0 = \infty$ is a regular singular point if the equation can be written as

$$z\frac{dU}{dz} = f(z^{-1})U$$

with f holomorphic in a small ball.

1. One pole. If there is one pole we can move it to ∞ by a Möbius transform and obtain a polynomial differential equation

   $$u'' = p(z)u' + q(z)u.$$

   ∞ is in general not a regular singular point.

2. Two poles. In this case one can move them to 0 and ∞. The equation becomes
$$u'' = z^{-j}(p(z)u' + q(z)u)$$
with polynomials p and q and $j \in \mathbb{N}$.

3. Three poles. Normalization by a Möbius transform moves them to 0, 1 and ∞. Multiplication by $z^{\alpha}(1-z)^{\beta}$ with $\alpha, \beta \in \mathbb{C}$ (taking out a suitable line) one can normalize the problem in the case of regular singular points to
$$z(1-z)\frac{d^2u}{dz^2} + [c-(a+b+1)z]\frac{du}{dz} - abu = 0 \tag{4.12}$$
with $a, b, c \in \mathbb{C}$. This is the hypergeometric differential equation.

Lemma 4.16. *The hypergeometric differential equation has a unique holomorphic solution near $z = 0$ with $u(0) = 1$. We denote it by*
$$F\begin{pmatrix} a & & b \\ & c & ; z \end{pmatrix} \tag{4.13}$$

Proof. We construct the solution by a power series. Then
$$F\begin{pmatrix} a & & b \\ & c & ; z \end{pmatrix} = 1 + \frac{ab}{c1!}z + \frac{a(a+1)b(b+1)}{c(c+1)2!}z^2 \dots$$
and it is not hard to see that the radius of convergence is 1. $\square$

Suppose that $c \neq 0$. Then a second solution is given by
$$z^{1-c}F\begin{pmatrix} a-c+1 & & b-c+1 \\ & 2-c & ; z \end{pmatrix}.$$

To see this we search a solution of the form $z^{1-c}v$. Then
$$\begin{aligned}
0 =& z(1-z)\frac{d^2(z^{1-c}v)}{dz^2} + [c-(a+b+1)z]\frac{d(z^{1-c}v)}{dz} - abz^{1-c}v \\
=& z^{1-c}\Big[z(1-z)v'' + 2(1-c)(1-z)v' - (1-c)c\frac{1-z}{z}v \\
& + [c-(a+b+1)z]v' + \frac{c(1-c)}{z}v - ((1-c)(a+b+1)+ab)v\Big] \\
=& z^{1-c}\Big[z(1-z)v'' + [(2-c)-(a+b-2c+3)z]v' + ((1-c)(c-1-a-b)-ab)v\Big] \\
=& z^{1-c}\Big\{z(1-z)\frac{d^2v}{dz^2} + [2-c-(a+b-2c+3)z]\frac{dv}{dz} - (a-c+1)(b-c+1)v\Big\}.
\end{aligned} \tag{4.14}$$

Equation (4.9) is a confluent hpyergeometric equation. It can be written as Kummer's confluent equation

$$z\frac{d^2u}{dz^2} + (b-z)\frac{du}{dz} - au = 0 \tag{4.15}$$

with $r = z/2$ and $a = l+1-\xi/2 = l+1-n$ is a nonpositive integer and $b = 2(l+1)$.

Lemma 4.17. *Suppose that b is not a negative integer. There is a unique holomorphic solution with $M(a,b;0) = 1$ near 0. It is denoted by $M(a,b;z)$. It is a polynomial if a is a negative integer. There is a second solution defined in $B_1(0)\backslash\{(-1,0]\}$ which is unbounded near 0 if $\operatorname{Re} b > 1$.*

Proof. This follows from

$$M(a,b;z) = 1 + \frac{a}{b}z + \frac{a(a+1)}{b(b+1)2!}z^2 \dots$$

The second part is an exercise. □

Now we check (4.9).

Lemma 4.18. *The solutions described in terms of the Laguere polynomials are the only solutions to (4.9) which lead to bounded eigenfunctions of the Schrödinger operator with negative energy.*

4.7 Selfadjointness of Schrödinger operators

The main theorem in this section is

Theorem 4.19. *Suppose that $d > 4$, $V \in L^{d/2} + L^\infty$ is a real potential. Then the Schrödinger operator*

$$\Psi \to -\Delta\Psi + V\Psi$$

defines a unitary evolution and a unitary operator with domain H^2. The same conclusion holds if $d \leqslant 3$ and $V \in L^2 + L^\infty$ and if $d = 4$ and $V \in L^p + L^\infty$ for some $p > 2$.

It immediately implies that the Schrödinger operator of the hydrogen atom is selfadjoint with domain H^2 since we can decompose

$$|x|^{-1} = \chi_{|x|\leqslant 1}|x|^{-1} + \chi_{|x|>1}|x|^{-1}.$$

The second term is bounded, and the first lies in $L^2(\mathbb{R}^3)$.

Definition 4.20. *Let A be a densely defined closed operator with domain $D(A)$. A densely defined operator B with domain $D(B) \supset D(A)$ is called A bounded if there exist constants a, b so that*

$$\|Bx\| \leqslant a\|Ax\| + b\|x\|.$$

Here a is called the A bound of the A bounded operator B.

By the triangle inequality

Lemma 4.21. *Suppose that B_j, $j = 1, 2$ are A bounded with A bounds a_j. Then $\alpha_1 B_1 + \alpha_2 B_2$ is A bounded with A bound at most $|\alpha_1|a_1 + |\alpha_2|a_2$. The space of A bounded operators is a vector space.*

Theorem 4.22 (Kato-Rellich)**.** *Suppose that A is selfadjoint with domain $D(A)$. Suppose that B is A bounded with A bound $a < 1$ and symmetric. Then $A + B$ with domain $D(A)$ is selfadjoint.*

Proof. Clearly $A+B$ with domain $D(A)$ is symmetric. We have to show that the deficiency indices are 0, or, equivalently, that $A + B \pm i\lambda$ is surjective for one $\lambda > 0$. We claim that

$$\lim_{\lambda\to\infty} \|B(A - i\lambda)^{-1}\| \leqslant a.$$

To see this

$$\|B(A - i\lambda)^{-1}x\| \leqslant a\|A(A - i\lambda)^{-1}x\| + b\|(A - i\lambda)^{-1}x\| \leqslant (a + b/\lambda)\|x\|$$

and the limit is at most a.

We choose λ so that

$$\|B(A \pm i\lambda)^{-1}\| < 1.$$

Then

$$(A + B \pm i\lambda) = (1 + B(A \pm i\lambda)^{-1})(A \pm i\lambda)$$

is surjective. □

Let $V \in (L^{d/2} + L^\infty)$. We write it as $V_0 + V_1$ with $V_0 \in L^{d/2}$ and $V_1 \in L^\infty$. Since $C_0^\infty(\mathbb{R}^d)$ is dense in $L^{d/2}$ we may assume that for a chosen $\varepsilon > 0$, $\|V_0\|_{L^{d/2}} < \varepsilon$. Clearly the multiplication by a bounded function is $-\Delta$ bounded with $a = 0$. It remains to show that the multiplication by an $L^{\frac{d}{2}}$ function is $-\Delta$ bounded. We recall the Sobolev inequality:

$$\|f\|_{L^p(\mathbb{R}^d)} \leqslant c\|\nabla f\|_{L^q(\mathbb{R}^d)}$$

for $1 \leqslant q < d$,

$$\frac{1}{p} + \frac{1}{d} = \frac{1}{q}.$$

We apply this twice to obtain

$$\|f\|_{L^p(\mathbb{R}^d)} \leqslant c\|D^2 f\|_{L^q(\mathbb{R}^d)}$$

provided $1 \leqslant q < \frac{d}{2}$

$$\frac{1}{p} + \frac{2}{d} = \frac{1}{q}.$$

Thus, if $d > 4$

$$\|V_0 u\|_{L^2(\mathbb{R}^d)} \leqslant \|V_0\|_{L^{\frac{d}{2}}} \|u\|_{L^{\frac{2d}{d-4}}} \leqslant \|V_0\|_{L^{\frac{d}{2}}} \|D^2 u\|_{L^2} < \varepsilon \|\Delta u\|_{L^2}.$$

For $d = 4$ we recall the Sobolev inequality for $2 \leqslant r < \infty$

$$\|u\|_{L^r(\mathbb{R}^4)} \leqslant c\|u\|_{H^2(\mathbb{R}^4)}$$

and for $d \leqslant 3$ we use Sobolev's inequality and Morrey's inequality

$$\|u\|_{L^\infty(\mathbb{R}^d)} \leqslant c\|u\|_{H^2(\mathbb{R}^d)}.$$

We equip H^2 with the norm

$$\|u\|_{H^2}^2 = \|(1+|k|^2)\hat{u}\|_{L^2}^2 = \|u\|_{L^2}^2 + \|\Delta u\|_{L^2}^2.$$

If $d \leqslant 3$ (the argument for $d = 4$ being similar), given $c_0 > 1$ there exists $c_1 > 0$ so that

$$\|\psi\|_{L^\infty} \leqslant c_0 \|\Delta \psi\|_{L^2} + c_1 \|\psi\|_{L^2},$$

and thus (without loss of generality we can assume also $\|V_0\|_{L^2} < \varepsilon$)

$$\|V_0 \psi\|_{L^2} \leqslant \|V_0\|_{L^2} \|\psi\|_{L^\infty} \leqslant c_0 \varepsilon \|\Delta \psi\|_{L^2} + c_1 \varepsilon \|\psi\|_{L^2}.$$

[23.06.2017]

[28.06.2017]

4.8 Eigenvalues of Schrödinger operators

We denote by $C_0(\mathbb{R}^d)$ the space of all continuous functions with limit 0 at infinity. We denote by $H^{-1}(\mathbb{R}^d)$ the dual space of $H^1(\mathbb{R}^d)$ with the norm

$$\|u\|_{H^1(\mathbb{R}^d)}^2 = \|u\|_{L^2(\mathbb{R}^d)}^2 + \||\nabla u|\|_{L^2(\mathbb{R}^d)}^2 = \int_{\mathbb{R}^d} (1+|k|^2)|\hat{u}|^2 dx$$

and

$$\|u\|_{H^{-1}(\mathbb{R}^d)}^2 = \int_{\mathbb{R}^d} (1+|k|^2)^{-1} |\hat{u}|^2 dx.$$

Theorem 4.23. *Suppose that $V \in L^{\frac{d}{2}}(\mathbb{R}^d) + C_0(\mathbb{R}^d)$ if $d \geqslant 3$, $V \in L^p(\mathbb{R}^2) + C_b(\mathbb{R}^2)$ if $d = 2$ with $p > 1$ and $V \in L^1(\mathbb{R}) + C_0(\mathbb{R})$ if $d = 1$. We consider the Schrödinger operator*

$$H^1 \ni \psi \to -\Delta\psi + V\psi \in H^{-1}$$

and call $z \in \mathbb{C}$ an eigenvalue if there exists $\psi \in H^1(\mathbb{R}^d)$ with

$$-\Delta\psi + V\psi = z\psi.$$

If z is an eigenvalue then $z \in \mathbb{R}$.

If ψ is an eigenfunction with eigenvalue $z < 0$ and if $0 < \kappa < \sqrt{-z}$ then there exist $C(z, \kappa, V)$ and R so that

$$\|e^{\frac{\kappa|x|}{2}}\psi\|_{L^2(\mathbb{R}^d)} + \|e^{\frac{\kappa|x|}{2}}\nabla\psi\|_{L^2(\mathbb{R}^d)} \leqslant C\|\psi\|_{L^2(B_R(0))}. \tag{4.16}$$

The set of eigenvalues is discrete in $(-\infty, 0)$. Every negative eigenvalue has finite multiplicity.

We observe that there exists C so that

$$C^{-1}\|e^{\kappa|x|/2}u\|_{H^1} \leqslant \|e^{\frac{\kappa|x|}{2}}u\|_{L^2} + \|e^{\frac{\kappa|x|}{2}}\nabla u\|_{L^2} \leqslant C\|e^{\kappa|x|/2}u\|_{H^1}$$

which is not hard to see and gives an equivalent expression for the left hand side of (4.16).

Proof. We begin with the observation that if

$$-\Delta\psi + V\psi = z\psi$$

then

$$\langle\nabla\psi, \nabla\phi\rangle + \langle V\psi, \phi\rangle = z\langle\psi, \phi\rangle$$

for all $\phi \in H^1$ and vice versa. In particular we may set $\phi = \psi$. Then both terms on the left hand side are real and hence z is real or $\psi = 0$.

Now let $\psi \in L^2$ be nonzero, $z < 0$ and

$$-\Delta\psi + V\psi = z\psi.$$

Let $h \in C_b^1([0, \infty))$ with $h(0) = 1$. We set $\phi = h(|x|)\psi$. Then

$$\begin{aligned} \mathrm{Re}\langle\nabla\psi, \nabla[h(|x|)\psi]\rangle &= \int h(|x|)|\nabla\psi|^2 dx + \frac{1}{2}\sum_j \int h'(|x|)\frac{x_j}{|x|}\partial_j|\psi|^2 dx \\ &= \int h(|x|)|\nabla\psi|^2 dx - \frac{1}{2}\int |\psi|^2 \sum_j \partial_j \frac{x_j h'(|x|)}{|x|} dx. \end{aligned}$$

We choose $h(|x|) = e^{\kappa |x|}$. Then

$$\frac{1}{2}\sum_{j=1}^d \partial_{x_j} \frac{\kappa x_j e^{\kappa|x|}}{|x|} = \frac{1}{2} e^{\kappa|x|}[\kappa^2 + \kappa \frac{d-1}{|x|}]$$

hence by $-\Delta\psi = z\psi - V\psi$ we have

$$\begin{aligned}&\int e^{\kappa|x|}|\nabla\psi|^2 - (z+\frac{1}{2}\kappa^2)\int e^{\kappa|x|}|\psi|^2 dx \\ &= -\int V e^{\kappa|x|}|\psi|^2 dx + \frac{1}{2}(d-1)\kappa \int e^{\kappa|x|}|x|^{-1}|\psi|^2 dx.\end{aligned}$$

We write

$$V = V_0 + V_1$$

with $\|V_0\|_{L^{\frac{d}{2}}} < \varepsilon$ if $d \geqslant 3$ (modifications for $d = 1, 2$ are an exercise) and $V_1 \in C_0(\mathbb{R}^d)$ and R so that $|V_1(x)| < \varepsilon$ for $|x| \geqslant R$ and $R^{-1} \leqslant \varepsilon$ for ε to be chosen. Then, as in the proof of Theorem 4.19, the right hand side is bounded by - pretending that $|x|^{-1}$ is bounded near zero -

$$C\varepsilon \int e^{\kappa\sqrt{1+|x|^2}}|\nabla\psi|^2 dx + C\|\psi\|^2_{L^2(B_R(0))} + 2\varepsilon \int e^{\kappa\sqrt{1+|x|^2}}|\psi|^2 dx.$$

The singularity at $x = 0$ can be avoided by replacing $|x|$ by $\sqrt{1+|x|^2}$ or the weight.

Assuming that the right hand side is bounded we subtract these terms from both sides and arrive at (4.16). To ensure this boundedness we choose

$$h(|x|) = e^{\kappa \frac{|x|}{1+\delta|x|}}$$

and then we let δ tend to 0. This completes the proof of (4.16).

As for selfadjoint operators we see that there are no generalized eigenfunctions and eigenfunctions to different eigenvalues are orthogonal. Let $\varepsilon > 0$, $z_j < -\varepsilon$ and ψ_j an orthonormal family of eigenfunctions to the eigenvalues z_j. We want to prove that there are at most finitely many ψ_j, which we prove by contradiction. We claim that ψ_j converges weakly to zero. Indeed,

$$\lim_{j\to\infty}\langle \psi_j, \psi_l\rangle = 0$$

for all l, hence the same is true on the span, and hence also on the closure of the span. This implies weak convergence. By (4.16) (which holds uniformly for all the eigenfunctions with eigenvalues below $-\varepsilon$) and Kolmogorovs criterion the sequence converges strongly in $L^2(\mathbb{R}^d)$. The limit is nonzero (since $\|\psi_j\|_{L^2} = 1$) and this is a contradiction (since we claimed $\psi_j \rightharpoonup 0$). $\square$

Normalized eigenfunctions to the eigenvalue z are called bound states for the energy z. The bound state to the lowest eigenvalue is called ground state.

There is not much we can say about a potential eigenvalue 0.

Theorem 4.24. *Suppose that $V \in L^\infty$ and there exist C and $s > 1$ so that*

$$|V(x)| \leqslant C|x|^{-s}.$$

Then there is no positive eigenvalue.

The strategy is the following:

1. We prove that such eigenfunctions have to have compact support.
2. The second step is called unique continuation: If a solution to a suitable homogeneous elliptic equation vanishes on an open set it has to be identically zero.

The proof consists of a number of arguments of independent interest. It is convenient to introduce conformal coordinates. We write

$$x = e^t y$$

with $|y| = 1$ and $t \in \mathbb{R}$ provided $x \neq 0$.

Lemma 4.25. *The following formula holds*

$$|x|^{\frac{2+d}{2}} \Delta(|x|^{\frac{2-d}{2}} u) = \partial_t^2 u + \Delta_{\mathbb{S}^{d-1}} u - \Big(\frac{d-2}{2}\Big)^2 u.$$

Proof. We write $x = ry$ with $r > 0$ and $|y| = 1$. Then with polar coordinates

$$\Delta w = \partial_r^2 w + \frac{d-1}{r}\partial_r w + \frac{1}{r^2}\Delta_{\mathbb{S}^{d-1}} w$$

and the statement is now a consequence of the chain rule. □

Now let $z = 1 > 0$. The restriction to $z = 1$ is unimportant but it simplifies the notation. The condition on V implies that for all ε there exists R so that

$$|V(x)| \leqslant \varepsilon/|x| \qquad \text{for } |x| \geqslant R.$$

We rewrite the equation $-\Delta\psi + V\psi = \psi$ as with $\psi = |x|^{\frac{2-d}{2}} v$

$$v_{tt} + \Delta_{\mathbb{S}^{d-1}} v - ((d-2)/2))^2 v + e^{2t} v - e^{2t} V(ty) v = 0. \tag{4.17}$$

We consider

$$v_{tt} + \Delta_{\mathbb{S}^{d-1}} v - ((d-2)/2))^2 v + e^{2t} v = f. \tag{4.18}$$

Lemma 4.26. *Suppose that $h' \geqslant \delta > 0$, $h'h'' \geqslant -\frac{1}{4}e^{2t}$ and $|h^{(3)}| \leqslant \frac{1}{4}e^{2t}$ and that $v(\cdot, y)$ is compactly supported in $(0,\infty)$. Then*

$$\|e^{h(t)+t} v\|_{L^2} \leqslant c\|e^{h(t)} f\|_{L^2}.$$

Proof. Let $w = e^{h(t)}v$ and $g = e^{h(t)}f$. By (4.18) it satisfies

$$w_{tt} - h'w_t - \partial_t(h'w) + \Delta_{\mathbb{S}^{d-1}} w - ((d-2)/2)^2 w + |h'|^2 w + e^{2t} w = g.$$

It suffices to prove the estimate for $w(t,y) = u(t)h_m(y)$, $g(t,y) = l(t)h_m(y)$ where h_m is a harmonic polynomial. This reduces the problem to

$$u'' - h'u' - (h'u)' - [(m + (d-2)/2)^2 - h'^2]u + e^{2t}u = l.$$

We multiply by u' and integrate and notice that u is compactly supported. Then

$$\begin{aligned}\int 2h'(u')^2 + e^{2t}|u|^2 =& \int -lu' + \frac{1}{2}h^{(3)}|u|^2 - h'h''|u|^2 \\ \leqslant& \|l\|_{L^2}\|u'\|_{L^2} + \frac{1}{2}\int e^{2t}|u|^2 dt.\end{aligned}$$

We subtract the second term from both sides and obtain

$$\int 2h'(u')^2 + \frac{1}{2}e^{2t}|u|^2 \leqslant \delta^{-1/2}\|l\|_{L^2}\delta^{1/2}\|u'\|_{L^2} \leqslant \frac{1}{2\delta}\|l\|_{L^2}^2 + \frac{\delta}{2}\|u'\|_{L^2}^2.$$

We subtract the second term from both sides and arrive at the desired inequality.

We used more regularity in the proof then we had assumed in the statement. This can be justified by regularizing v first. □

[28.06.2017]

[30.06.2017]

We can easily relax the condition of compact support, but we want to keep that 0 is not in the support.

We return to the transformed equation (4.17) and define for an $R > 0$ to be chosen later

$$w = \eta(t-R)v$$

where $\eta(s) = 1$ for $s \geqslant 1$ and $\eta(s) = 0$ for $s \leqslant 0$. It satisfies (4.18) with

$$f = e^{2t}Vw + 2\eta'(t-R)v' + \eta''(t-R)v.$$

By Lemma 4.26 and the monotonicity of h, there exists a constant C depending on $\|\psi\|_{H^1}$ such that

$$\|e^h e^t w\|_{L^2} \leqslant C(e^{h(R+1)} + \|e^h e^{2t} V w\|).$$

We choose R large so that

$$e^t |V(e^t y)| \leqslant 1/(2C), \quad \text{for } t \geqslant R,$$

so that we can absorb the V term on the right hand side by the left hand side. Then

$$\|e^h e^t w\|_{L^2} \leqslant C e^{h(R+1)}.$$

We will see that we may choose $h = \tau t$ with $\tau > 0$. Then

$$\|e^{(\tau+1)(t-R-1)} w\|_{L^2} \leqslant C$$

in particular

$$\|w\|_{L^2(\{t \geqslant R+2\})} \leqslant C e^{-\tau} \to 0 \qquad \text{for } \tau \to \infty.$$

This implies that ψ has compact support provided we show that we can do the argument without get unbounded terms. There are two points to add:

$$h(t) = \tau \frac{t}{1 + \varepsilon_0 t} \tag{4.19}$$

and let $\varepsilon_0 \to 0$. We notice

$$\|\psi\|_{L^2(\mathbb{R}^d)} = \|e^{\frac{1}{2}t} v\|_{L^2(\mathbb{R} \times \mathbb{S}^{d-1})} \tag{4.20}$$

and we apply the argument with the above h and a truncation at large t to obtain the estimate of Lemma 4.26 without the truncation at infinity.

Theorem 4.27. *Suppose that $\psi \in H^1$ satisfies*

$$-\Delta \psi + V \psi = 0, \quad V \text{ bounded,}$$

in an open connected set U. If ψ vanishes in an open set then it vanishes on U.

Proof. We argue similar to above and consider

$$-v_{tt} - \Delta_{\mathbb{S}^{d-1}} v + ((d-2)/2)^2 v = f$$

and claim that

$$\|e^{\tau t} v\|_{L^2} \leqslant \|e^{\tau t} f\|_{L^2} \tag{4.21}$$

for all $\tau \in \frac{1}{2}\mathbb{Z}+\frac{1}{4}$ and v with compact support. As above it suffices to consider $v = \tilde{v}(t)h_m(y)$ and $w = e^{\tau t}\tilde{v}(t)$. We write it as

$$-w'' + 2\tau w' + [(m + (d-2)/2)^2 - \tau^2]w = g,$$

which can be rewritten as

$$(-\frac{d}{dt} + \kappa + \tau)(\frac{d}{dt} + \kappa - \tau)w = g, \quad \kappa = m + (d-2)/2.$$

Suppose that $g \in L^2$. We claim that there is a unique $w_1 \in H^1$ so that

$$(-\frac{d}{dt} + (\kappa + \tau))w_1 = g.$$

Uniqueness is easy: If $g = 0$ and $w_1 = ce^{(\kappa+\tau)t}$ and it is in $L^2(\mathbb{R})$ only if $c = 0$. Suppose that $\kappa < -\tau$. Then

$$w_1(t) = -\int_{-\infty}^{t} e^{(\kappa+\tau)(t-s)} g(s)ds,$$

and by Schur's estimate

$$\begin{aligned}\|w_1\|_{L^2} \leqslant& \max\Big\{\sup_t \int_{-\infty}^{t} e^{(\kappa+\tau)(t-s)}ds, \sup_s \int_s^{\infty} e^{(\kappa+\tau)(t-s)}dt\Big\}\|g\|_{L^2}\\ \leqslant& |\kappa+\tau|^{-1}\|g\|_{L^2}.\end{aligned}$$

Then $\frac{1}{|\kappa+\tau|} \leqslant 4$ if $\tau \in \frac{1}{4} + \frac{1}{2}\mathbb{Z}$. The case $\kappa > -\tau$ is similar with $w_1(t) = \int_t^{\infty} e^{(\kappa+\tau)(t-s)}g(s)ds$. It remains to study

$$(\frac{d}{dt} + \kappa - \tau)w = w_1$$

which follows by the same arguments. Estimate (4.21) is equivalent to

$$\||x|^{\tau}\psi\|_{L^2} \leqslant c\||x|^{2+\tau}\Delta\psi\|_{L^2} \tag{4.22}$$

for $\tau \in \frac{1}{2}\mathbb{Z} + \frac{1}{4}$ and ψ with compact support.

Suppose that ψ has compact support, that $0 \in U$ is outside the support and define $\rho = \operatorname{dist}\{0, \operatorname{supp}\psi\}$. We assume that ρ is small and $B_{4\rho}(0) \subset U$, which holds by translation invariance of the problem. We want to reach a contradiction. Let $\eta \in C^{\infty}$ satisfy $\eta(r) = 1$ for $r \leqslant 1$, $\eta(r) = 0$ for $r \geqslant \frac{3}{2}$ and define

$$u = \eta(|x|/(2\rho))\psi(x).$$

Then

$$-\Delta u = -Vu - 2\nabla(\eta(|x|/(2\rho))) \cdot \nabla\psi - \Delta(\eta(|x|/(2\rho)))\psi$$

and, for $\tau \in \frac{1}{2}\mathbb{Z} + \frac{1}{4}$,

$$\||x|^\tau u\|_{L^2} \leqslant C\||x|^{\tau+2}Vu\|_{L^2} + C(\psi,\rho)(3\rho)^\tau.$$

Since

$$\||x|^{\tau+2}Vu\|_{L^2} \leqslant (4\rho)^2\|V\|_{L^\infty}\||x|^\tau u\|_{L^2}$$

can be absorbed by the left hand side if ρ is sufficiently small which we may assume. Then

$$\|u\|_{L^2(B_{2\rho}(0))} \leqslant C(\frac{3}{2})^{\tau_j} \to 0$$

for a sequence $\tau_j \in \frac{1}{4} + \frac{1}{2}\mathbb{Z}$ with $\tau_j \to -\infty$. Thus $u|_{B_{2\rho}(0)} = \psi|_{B_{2\rho}(0)} = 0$, contradicting our assumptions.

$\square$

This technique goes back to Carleman and the inequalities of the Lemmas are called Carleman inequalities.

Lemma 4.28. *Let V be a continuous real potential which satisfies the assumptions of Theorem 4.23. Then $\chi_{(-\infty,0)}(-\Delta+V)$ is the sum of the projections to eigenspaces with negative eigenvalues.*

Proof. Assume that there is $\phi \in H^1$ so that $\langle(-\Delta+V)\phi,\phi\rangle < 0$. Otherwise

$$A(\phi) = \sum_{j=1}^d \|\partial_{x_j}\phi\|_{L^2}^2 + \int V|\phi|^2 dx \geqslant 0, \quad \forall \phi \in H^1,$$

and $\sigma(-\Delta+V) \subset [0,\infty)$.

We have seen that there exists C such that

$$\langle(-\Delta+V)\phi,\phi\rangle \geqslant -C\|\phi\|_{L^2}^2.$$

Now let ϕ_j be a minimizing sequence with $\|\phi_j\|_{L^2} = 1$ and

$$\langle(-\Delta+V)\phi_j,\phi_j\rangle \leqslant -\varepsilon.$$

Then, as for previous proofs in the subsection,

$$\|\nabla\phi_j\|_{L^2}^2 = \langle(-\Delta+V)\phi_j,\phi_j\rangle - \int V|\phi_j|^2 dx \leqslant -\varepsilon + 1/2\|\nabla\phi_j\|_{L^2}^2 + C(V)\|\phi_j\|_{L^2}^2$$

and hence there exists C so that $\|\phi_j\|_{H^1} \leqslant C$. We may assume that ϕ_j converges weakly in H^1 to ϕ. For every continuous V_1 the sequence $\phi_j|_{\operatorname{supp} V_1}$ converges in L^2 by the compactness of the embedding $H^1(B_R(0)) \to L^2(B_R(0))$. Thus

$$\lim_{j\to\infty} \int V|\phi_j|^2 dx$$

exists and is nonzero. Moreover

$$\|\nabla\phi\| \leqslant \liminf \|\nabla\phi_j\|$$

and the same holds for the L^2 norm. The limit cannot be trivial. We rescale the L^2 norm to 1 which decreases

$$\langle(-\Delta + V)\phi, \phi\rangle.$$

Since we had a minimizing sequence, the rescaling factor had to be 1 and $\phi_j \to \phi$ in H^1. ϕ satisfies the Euler-Lagrange equation

$$-\Delta\phi + V\phi = z\phi$$

for some $z < 0$. But then

$$\langle(-\Delta + V)\phi, \phi\rangle = z$$

and z is the energy.

We repeat the procedure in $\phi^\perp$ if there is a perpendicular function with negative energy. This yields an orthonormal sequence of eigenfunctions. There can be only finitely many until the energy in the orthogonal complement is above $-\varepsilon$. □

[30.06.2017]

[05.07.2017]

5 Scattering

In this section we will consider real potentials $V \in L^2 + L^\infty$. We will add conditions whenever needed. We know that $-\Delta + V$ is selfadjoint with real spectrum. We will see that under suitable assumptions

1. $[0, \infty)$ is in the spectrum.

2. Let $P : L^2(\mathbb{R}^d) \to W$ be the projection corresponding to the multiplication by $\chi_{(0,\infty)}(-\Delta + V)$. Then there exists a unitary operator $U : L^2 \to W$ so that
$$Ue^{it\Delta} = e^{it(\Delta - V)}U$$

3. We have seen that there is an at most countable set of negative eigenvalues with 0 the only possible accumulation point.

4. Sometimes it is possible to replace the characteristic function above by $\chi_{[0,\infty)}(-\Delta + V)$.

The resolvent and the evolutions are connected through the formula of the next lemma.

Lemma 5.1. *Let X be a Hilbert space and T be a selfadjoint operator on X. Let $\eta \in C(\mathbb{R})$ with compact support. Then*

$$\langle \eta(T)\phi, \phi\rangle = \pm\frac{1}{\pi}\lim_{\varepsilon\to 0}\operatorname{Im}\int_{\mathbb{R}} \eta(\lambda)\langle (T - \lambda \mp i\varepsilon)^{-1}\phi, \phi\rangle d\lambda$$

Proof. By the spectral theorem it suffices to consider $X = L^2(\mu)$ for a probability measure μ on $\mathbb{R}$ and $T = M_x$ the multiplication operator by x.

Then we have to show that

$$\begin{aligned}
&\pm\frac{1}{\pi}\lim_{\varepsilon\to 0}\operatorname{Im}\int_{\mathbb{R}\times\mathbb{R}} \eta(\lambda)(x - \lambda \mp i\varepsilon)^{-1}|\phi(x)|^2 d\mu(x) d\lambda \\
=&\lim_{\varepsilon\to 0}\int_{\mathbb{R}} |\phi(x)|^2 \int_{\mathbb{R}} \frac{1}{\pi}\frac{\varepsilon}{|x-\lambda|^2 + \varepsilon^2}\eta(\lambda) d\lambda d\mu(x) \\
=&\int_{\mathbb{R}} \eta(x)|\phi(x)|^2 d\mu(x) = \langle \eta\phi, \phi\rangle_{L^2(\mu)}.
\end{aligned}$$

∎

It is not difficult to extend this proof to $\eta(x) = e^{itx}$ and we obtain a similar formula for the generated group e^{itT}. It is tempting to try to study the limit
$$\lim_{\varepsilon\to 0}(T - \lambda \mp i\varepsilon 1)^{-1}$$
and we will see that this is possible for $T = -\Delta$ and many Schrödinger operators $-\Delta + V$. We will also relate the limit of the resolvents of the two operators via the Lippmann-Schwinger equation.

5.0.1 The spectrum of Schrödinger operators

We recall that up to conjugation by a unitary operator every densely defined selfadjoint operator can be realized as multiplication by x in some $L^2(\mu)$ where μ is an at most countable sequence of measures. For $\phi \in X$ we define X_ϕ the closure of the span of powers of the Cayley transform and its conjugate to ϕ. By Theorem 3.32 there exists a unique probability measure μ and a unitary map $U : L^2(\mu) \to X_\phi$ with

$$U(1) = \phi, \qquad U(xf) = TU(f).$$

Definition 5.2. *Let T be a densely defined operator. We call $\lambda \in \mathbb{C}$* eigenvalue *with eigenfunction $\psi \in D(T)$ if $T\psi = \lambda\psi$.*

Now assume that T is selfadjoint. The continuous spectrum *is the set of all $\lambda \in \mathbb{R}$ in the spectrum so that for all ϕ the measure μ_ϕ (the measure corresponding to $T - \lambda$ on the span of $C^j\phi$ and $(C^j)^*\phi$ where C is the Caley transform of $T - \lambda$) is absolutely continuous with respect to the Lebesgue measure. The* singular spectrum *is the complement of the discrete and the continuous spectrum in the spectrum.*

5.1 The wave operators

Let X be a Hilbert space (to free the letter H for Schrödinger operators). Let H_0 be a selfadjoint operator. Let H be a second selfadjoint operator. We denote the generated groups by e^{-itH_0} resp. e^{-itH}. We recall that $e^{it\Delta}\psi_0$ is the solution to

$$i\partial_t\psi + \Delta\psi = 0, \qquad \psi(0) = \psi_0.$$

We keep in mind the example that $H_0 = -\Delta$ and $H = -\Delta + V$ with some suitable potential V.

Definition 5.3. *We define the domain of the wave operators $D(W_\pm)$ by*

$$D(W_\pm) = \{\psi \in X : \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\psi \text{ exists } \}$$

and for $\psi \in D(W_\pm)$

$$W_\pm\psi = \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\psi.$$

We say that $D(W_+)$ is the set of all incoming states *and $D(W_-)$ is the set of all* outgoing states. *If $\psi \in \operatorname{Ran} W_- \cap \operatorname{Ran} W_+$ we call it a* scattering state.

Clearly

$$\|W_\pm \psi\| = \lim_{t\to\pm\infty} \|e^{itH}e^{-itH_0}\psi\| = \|\psi\|$$

and hence $D(W_\pm)$ is closed. A similar argument shows that $\operatorname{Ran} W_\pm$ is closed.

Lemma 5.4. *The sets* $D(W_\pm)$ *and* $\operatorname{Ran} W_\pm$ *are closed and*

$$W_\pm : D(W_\pm) \to \operatorname{Ran} W_\pm$$

is unitary. Moreover

$$W_\pm e^{-itH_0}\psi = e^{-itH}W_\pm\psi, \quad \psi \in D(W_\pm). \tag{5.1}$$

Proof. Let ψ_j be a Cauchy sequence in $D(W_+)$. Then

$$\|e^{itH}e^{-itH_0}(\phi_j - \phi_l)\| = \|\phi_j - \phi_l\|$$

and

$$\lim_{t\to+\infty} e^{itH}e^{-itH_0}(\phi_j - \phi_l)$$

is a Cauchy sequence. Thus $D(W_+)$ is closed. And $W_+ : D(W_+) \to \operatorname{Ran} W_+$ is unitary:

$$(e^{itH_0}e^{-itH})(e^{itH}e^{-itH_0})\phi = \phi, \text{ and } W_\pm^*\psi = \lim_{t\to\pm\infty} e^{itH_0}e^{-itH}\psi.$$

Hence $\operatorname{Ran} W_+$ is closed. The same argument applies to W_-. Finally

$$W_+e^{-itH_0}\psi = \lim_{s\to\infty} e^{isH}e^{-i(s+t)H_0}\psi = \lim_{s\to\infty} e^{i(s-t)H}e^{-isH_0}\psi = e^{-itH}W_+\psi$$

under the assumption on ψ. $\square$

In particular $D(W_\pm)$ is invariant under e^{itH_0} and $\operatorname{Ran} W_\pm$ is invariant under e^{itH}. Hence by differentiating (5.1) with respect to t we also have

$$W_\pm H_0\psi = HW_\pm\psi$$

for $\psi \in D(H_0) \cap D(W_\pm)$. We define the scattering operator

$$S = W_-^*W_+, \quad W_-^* = \lim_{t\to-\infty} e^{itH_0}e^{-itH}$$

with domain $\{\psi \in D(W_+) : W_+\psi \in \operatorname{Ran} W_-\}$.

Lemma 5.5 (Cook)**.** *Suppose that $D(H_0) \subset D(H)$. If*

$$\int_0^\infty \|(H - H_0)e^{\mp itH_0}\psi\| < \infty$$

then $\psi \in D(W_\pm)$. In this case

$$\|W_\pm\psi - \psi\| \leqslant \int_0^\infty \|(H - H_0)e^{\mp itH_0}\psi\| dt.$$

Proof. We write

$$\begin{aligned}
\langle e^{itH}e^{-itH_0}\psi, \phi\rangle =& \langle \psi, \phi\rangle + \int_0^t \frac{d}{ds}\langle e^{isH}e^{-isH_0}\psi, \phi\rangle ds \\
=& \langle \psi, \phi\rangle + i\int_0^t \langle e^{isH}(H - H_0)e^{-isH_0}\psi, \phi\rangle ds \\
=& \langle \psi, \phi\rangle + i\int_0^t \langle (H - H_0)e^{-isH_0}\psi, e^{-isH}\phi\rangle ds
\end{aligned}$$

and

$$\Big|\int_0^\infty \langle (H - H_0)e^{-isH_0}\psi, e^{-isH}\phi\rangle ds\Big| \leqslant \|\phi\| \int_0^\infty \|(H - H_0)e^{-itH_0}\psi\| dt.$$

This completes the proof. $\square$

Theorem 5.6. *Let $d = 3$. Suppose that H_0 is the free Schrödinger operator, $H = H_0 + V$, $V \in L^2(\mathbb{R}^3)$. Then $D(W_\pm) = L^2(\mathbb{R}^3)$.*

Proof. Since $L^1 \cap H^3$ is dense in L^2 and $D(W_\pm)$ is closed, it suffices to show $L^1 \cap H^3 \subset D(W_\pm)$. If $\psi \in L^1 \cap H^3$ then by Lemma 4.2 and Sobolev's embedding $H^3(\mathbb{R}^3) \hookrightarrow C_b(\mathbb{R}^3)$ we have

$$\begin{aligned}
\int_0^\infty \|Ve^{it\Delta}\psi\|_{L^2} dt \leqslant& \|V\|_{L^2} \int_0^\infty \|e^{it\Delta}\psi\|_{L^\infty} dt \\
\leqslant& \|V\|_{L^2}\Big[\int_1^\infty (4\pi t)^{-\frac{3}{2}} dt \|\psi\|_{L^1(\mathbb{R}^3)} + \sup_{0\leqslant t\leqslant 1} \|e^{it\Delta}\psi\|_{L^\infty(\mathbb{R}^3)}\Big] \\
\leqslant& c\|V\|_{L^2}\Big[\|\psi\|_{L^1(\mathbb{R}^3)} + \sup_{0\leqslant t\leqslant 1} \|e^{it\Delta}\psi\|_{H^3(\mathbb{R}^3)}\Big].
\end{aligned}$$

Since derivatives of solutions to the free Schrödinger equation are again solutions to the free Schrödinger equation, we know

$$\|e^{it\Delta}\psi\|_{H^3} = \|\psi\|_{H^3}.$$

Thus by Lemma 5.5, $\psi \in D(W_\pm)$. $\square$

This is not sufficient to cover the hydrogen Schrödinger operator and even the statement requires a modification for that operator. The modification is called long range scattering and occurs already for classical Coulomb scattering.

5.2 The case of one space dimension

In this section we want to study the structure of the problem in the simplest possible setting. We consider the Schrödinger operator

$$-\psi'' + V\psi$$

where $V \in L^2(\mathbb{R})$ is assumed to have compact support and the solutions to

$$-\psi'' + V\psi = z\psi + f.$$

The resolvent of the *free* equation $-\psi'' - z\psi = f$ is (recalling (4.3))

$$(R_0(z)f)(x) = \frac{i}{2\sqrt{z}} \int_{\mathbb{R}} e^{i\sqrt{z}|x-y|} f(y)dy, \tag{5.2}$$

where we take the square root $\sqrt{z}$ with the positive imaginary part if $\operatorname{Im} z \neq 0$ so that the exponential decays as $x \to \pm\infty$. We write

$$R_0(\lambda \pm i0)f = \lim_{\varepsilon\to 0, \pm\varepsilon>0} R_0(\lambda + i\varepsilon)f \tag{5.3}$$

if $\lambda > 0$ for $f \in L^2_{comp}$ with compact support. Then $R_0(\lambda \pm i0) : L^2_{comp} \to L^2_{loc}$.

We denote by L^2_{comp} the L^2 functions with compact support and by L^2_{loc} the functions such that the restriction to open bounded sets are in L^2. We use the same indices also for other function spaces.

Lemma 5.7. *Suppose that $\lambda > 0$ and that $u \in C^2_b$ satisfies*

$$-\partial_{xx} u = \lambda u \qquad \textit{in } \mathbb{R}. \tag{5.4}$$

Then there exists $v_\pm$ so that

$$\hat{u}(\xi) = v_+ \delta_{\sqrt{\lambda}}(\xi) + v_- \delta_{-\sqrt{\lambda}}(\xi).$$

Moreover

$$\lim_{R\to\infty} \frac{1}{2r} \int_{-r}^{r} |u|^2 dx = (2\pi)^{-1}(|v_-|^2 + |v_+|^2),$$

and for $f_1, f_2 \in L^2_{comp}$,

$$\begin{aligned}
&\lim_{r\to\infty}\frac{1}{2r}\int_{-r}^{r} R(\lambda\pm i0)f_1\overline{R(\lambda\pm i0)f_2}dx \\
&=\frac{\pi}{4\lambda}\big(\hat f_1(\sqrt{\lambda})\overline{\hat f_2(\sqrt{\lambda})}+\hat f_1(\sqrt{-\lambda})\overline{\hat f_2(\sqrt{-\lambda})}\big),
\end{aligned} \tag{5.5}$$

$$\lim_{r\to\infty}\frac{1}{2r}\int_{-r}^{r} R(\lambda\pm i0)f_1\overline{R(\lambda\mp i0)f_2}dx=0,$$

$$\lim_{r\to\infty}\frac{1}{2r}\int_{-r}^{r} R(\lambda\pm i0)f_1\bar u dx=\pm\frac{i}{4\sqrt{\lambda}}\big(\hat f_1(\sqrt{\lambda})\overline{v_+}+\hat f_1(-\sqrt{\lambda})\overline{v_-}\big).$$

Proof. It follows from (5.4) that $\hat u$ is supported in $\pm\sqrt{\lambda}$ and hence it can be written as

$$\hat u=\sum_{k=n}^{N} a_n\big(\frac{d}{dk}\big)^n\delta_{\sqrt{\lambda}}+b_n\big(\frac{d}{dk}\big)^n\delta_{-\sqrt{\lambda}}$$

and

$$u=(2\pi)^{-\frac12}\sum_{n=0}^{N}\Big(a_n(-ix)^n e^{ix\sqrt{\lambda}}+b_n(-ix)^n e^{-ix\sqrt{\lambda}}\Big).$$

Since u is bounded by assumption, its Fourier transform is a sum of Dirac measure and hence $N=0$ and we take $v_+=a_0$, $v_-=b_0$ such that

$$u(x)=(2\pi)^{-\frac12}(v_+e^{ix\sqrt{\lambda}}+v_-e^{-ix\sqrt{\lambda}}).$$

Then

$$\frac{1}{2r}\int_{-r}^{r}|u|^2dx=(2\pi)^{-1}(|v_+|^2+|v_-|^2)+\frac{1}{2r}\operatorname{Re}(v_+\overline{v_-}\int_{-r}^{r}e^{2ix\sqrt{\lambda}}dx)$$

and since

$$\int_{-r}^{r}e^{2ix\sqrt{\lambda}}dx=\frac{1}{\sqrt{\lambda}}\operatorname{Im}e^{2ir\sqrt{\lambda}}$$

the first identity follows.

[05.07.2017]

[07.07.2017]

For the second equality, we first notice

$$\begin{aligned}
e^{-i\sqrt{\lambda}x}R(\lambda+i0)f_1(x)=&\frac{i}{2\sqrt{\lambda}}e^{-i\sqrt{\lambda}x}\int e^{i\sqrt{\lambda}(x-y)}f_1(y)dy\\
=&(2\pi)^{\frac12}\frac{i}{2\sqrt{\lambda}}\hat f_1(\sqrt{\lambda})
\end{aligned}$$

if f_1 has compact support and x is sufficiently large. Similarly, if $-x$ is large enough then

$$\begin{aligned} e^{i\sqrt{\lambda}x}R(\lambda+i0)f_1(x) =&\frac{i}{2\sqrt{\lambda}}e^{i\sqrt{\lambda}x}\int e^{-i\sqrt{\lambda}(x-y)}f_1(y)dy \\ =&(2\pi)^{\frac{1}{2}}\frac{i}{2\sqrt{\lambda}}\hat{f}_1(-\sqrt{\lambda}). \end{aligned}$$

Notice also that if we have the convergence

$$\lim_{x\to\infty} g(x) = c,$$

then we know

$$\lim_{r\to\infty}\frac{1}{r}\int_0^r g(y)dy = c,$$

since for any positive big enough real number r_0

$$\frac{1}{r}\int_0^r (g(y)-c)dy = \frac{1}{r}\int_0^{r_0}(g(y)-c)dy + \frac{1}{r}\int_{r_0}^r (g(y)-c)dy,$$

where as $r\to\infty$ the first term converges to 0 and the second term is bounded uniformly by $|g|_{[r_0,r]}-c|$ and hence converges to 0 by $g(y)\to c$. Now we calculate the second equality:

$$\begin{aligned} &\lim_{r\to\infty}\frac{1}{2r}\int_0^r R_0(\lambda+i0)f_1\overline{R_0(\lambda+i0)f_2}dx \\ &= \frac{1}{2}\lim_{x\to\infty}(R_0(\lambda+i0)f_1)(x)\overline{R_0(\lambda+i0)f_2}(x) \\ &= \frac{1}{2}\frac{1}{4\lambda}\lim_{x\to\infty} e^{-i\sqrt{\lambda}x}\int_{\mathbb{R}} e^{i\sqrt{\lambda}(x-y)}f_1(y)dy\,\overline{e^{-i\sqrt{\lambda}x}\int_{\mathbb{R}} e^{i\sqrt{\lambda}(x-\tilde{y})}f_2(\tilde{y})d\tilde{y}} \\ &= \frac{\pi}{4\lambda}\hat{f}_1(\sqrt{\lambda})\overline{\hat{f}_2(\sqrt{\lambda})}. \end{aligned}$$

The integral on $[-r,0]$ gives then $\frac{\pi}{4\lambda}\hat{f}_1(-\sqrt{\lambda})\overline{\hat{f}_2(-\sqrt{\lambda})}$.

It also implies the third equality. We restrict to the integral from $(0,\infty)$

$$\begin{aligned} &\lim_{r\to\infty}\frac{1}{2r}\int_0^r R(\lambda+i0)f_1\overline{R(\lambda-i0)f_2}dx \\ &= -\frac{\pi}{2\lambda}\lim_{r\to\infty}\frac{1}{2r}\int_0^r e^{2i\sqrt{\lambda x}}dx\,\hat{f}_1(\sqrt{\lambda})\overline{\hat{f}_2(\sqrt{-\lambda})} \\ &= 0. \end{aligned}$$

The fourth equality is similar: We combine the argument for the first and the second equality

$$\begin{aligned}
&\lim_{r\to\infty}\frac{1}{2r}\int_0^r R(\lambda-i0)f_1\bar{u}dx\\
&=-\lim_{r\to\infty}\frac{1}{2r}\int_0^r\frac{i}{2\sqrt{\lambda}}\int e^{-i\sqrt{\lambda}(x-y)}f_1(y)dy(2\pi)^{-\frac{1}{2}}(\overline{v_+}e^{-i\sqrt{\lambda}x}+\overline{v_-}e^{i\sqrt{\lambda}x})dx\\
&=-\frac{i}{4\sqrt{\lambda}}\hat{f}_1(-\sqrt{\lambda})\overline{v_-}.
\end{aligned}$$

□

Theorem 5.8. *Let $\lambda > 0$, $f \in L^2(\mathbb{R})$ with compact support and assume that $u \in H^1_{loc}(-R, R)$ satisfies*

$$-\frac{d^2}{dx^2}u-\lambda u=f.$$

Let

$$u_\mp := u - R_0(\lambda \pm i0)f.$$

Then

$$-\frac{d^2}{dx^2}u_\mp=\lambda u_\mp$$

and suppose $\hat{u}_\pm = u_{\pm,+}\delta_{\sqrt{\lambda}} + u_{\pm,-}\delta_{-\sqrt{\lambda}}$, then

$$|u_{+,+}|^2+|u_{+,-}|^2-|u_{-,+}|^2-|u_{-,-}|^2=\frac{\pi}{\sqrt{\lambda}}\operatorname{Im}\int u\bar{f}dx. \tag{5.6}$$

Proof. We define

$$u_0 = u - \frac{1}{2}(R_0(\lambda+i0)f + R_0(\lambda-i0))f,$$

then

$$u_\pm = u_0 \pm \frac{1}{2}(R_0(\lambda+i0)f - R_0(\lambda-i0))f.$$

Since $(-\partial_x^2-\lambda)R_0(\lambda\pm i0)f = f$, we have again

$$-\frac{d}{dx}^2 u_0=\lambda u_0,$$

and we define $u_{0,\pm}$ the same way as $u_{+,\pm}$, $u_{-,\pm}$. Noticing

$$\overline{\int(R_0(\lambda+i0)f)\bar{f}dx}=\int(R_0(\lambda-i0)f)\bar{f}dx,$$

approximating by smooth functions and using unitarity of the Fourier transform

$$\begin{aligned}\operatorname{Im}\int u\bar{f}dx &= \operatorname{Im}\int u_0\bar{f}dx = \operatorname{Im}\int \hat{u}_0\bar{\hat{f}}d\xi \\ &= \operatorname{Im}\Big[u_{0,+}\overline{\hat{f}(\sqrt{\lambda})} + u_{0,-}\overline{\hat{f}(-\sqrt{\lambda})}\Big].\end{aligned} \tag{5.7}$$

We claim that

$$\lim_{\varepsilon\to 0}[(|k|^2-(\lambda+i\varepsilon))^{-1}-(|k|^2-(\lambda-i\varepsilon))^{-1}] = \frac{\pi}{\sqrt{\lambda}}i(\delta_{\sqrt{\lambda}}+\delta_{-\sqrt{\lambda}}) \tag{5.8}$$

as distributions. To see this we assume that ϕ is a Schwartz function and we compute for $\varepsilon > 0$

$$\int\Big[\frac{1}{|k|^2-(\lambda+i\varepsilon)}-\frac{1}{|k|^2-(\lambda-i\varepsilon)}\Big]\phi(k)dk = \int_0^\infty ..dk + \int_{-\infty}^0 \dots dk$$

and

$$\int_0^\infty \dots dk = \frac{1}{2\sqrt{\lambda}}\int_0^\infty\Big[\frac{1}{k-\sqrt{\lambda+i\varepsilon}}-\frac{1}{k+\sqrt{\lambda-i\varepsilon}}\Big]\phi(k)dk + O(\varepsilon)$$

since for $k \geqslant 0$

$$\left|\frac{1}{k^2-(\lambda+i\varepsilon)}-\frac{1}{k^2-(\lambda-i\varepsilon)}-\frac{1}{2\sqrt{\lambda}}\Big[\frac{1}{k-\sqrt{\lambda+i\varepsilon}}-\frac{1}{k+\sqrt{\lambda-i\varepsilon}}\Big]\right| \leqslant C\varepsilon.$$

Now $\sqrt{\lambda\pm i\varepsilon} = \sqrt{\lambda}(\pm 1 + i\frac{\varepsilon}{2\lambda}) + O(\varepsilon^2)$,

$$\Big[\frac{1}{k-\sqrt{\lambda+i\varepsilon}}-\frac{1}{k+\sqrt{\lambda-i\varepsilon}}\Big] = \frac{2i\varepsilon/2\sqrt{\lambda}}{(k-\sqrt{\lambda})^2+\frac{\varepsilon^2}{4\lambda}} + O(\varepsilon^2).$$

Hence (5.8) follows:

$$\begin{aligned}&\lim_{\varepsilon\to 0}\frac{i}{\sqrt{\lambda}}\int_0^\infty\frac{\varepsilon}{(k-\sqrt{\lambda})^2+\varepsilon^2}\phi(k)dk \\ &= \lim_{\varepsilon\to 0}\frac{\pi i}{\sqrt{\lambda}}\int_{-\infty}^\infty\frac{1}{\pi}\frac{\varepsilon}{(k-\sqrt{\lambda})^2+\varepsilon^2}\phi(k)dk - \lim_{\varepsilon\to 0}\frac{i}{\sqrt{\lambda}}\int_{-\infty}^0\frac{\varepsilon}{(k-\sqrt{\lambda})^2+\varepsilon^2}\phi(k)dk \\ &= \frac{\pi i}{\sqrt{\lambda}}\phi(\sqrt{\lambda}).\end{aligned}$$

We rewrite identity (5.8) as

$$R_0(\lambda+i0)f - R_0(\lambda-i0)f = \frac{\sqrt{2\pi}}{2\sqrt{\lambda}}i\Big[e^{ix\sqrt{\lambda}}\hat{f}(\sqrt{\lambda}) + e^{-ix\sqrt{\lambda}}\hat{f}(-\sqrt{\lambda})\Big]$$

Thus
$$\hat{u}_\pm = \hat{u}_0 \pm \frac{\pi i}{2\sqrt{\lambda}}\Big(\hat{f}(\sqrt{\lambda})\delta_{\sqrt{\lambda}} + \hat{f}(-\sqrt{\lambda})\delta_{-\sqrt{\lambda}}\Big),$$
and
$$u_{\pm,+} = u_{0,+} \pm \frac{\pi i}{2\sqrt{\lambda}}\hat{f}(\sqrt{\lambda}),$$
$$u_{\pm,-} = u_{0,-} \pm \frac{\pi i}{2\sqrt{\lambda}}\hat{f}(-\sqrt{\lambda}).$$
Equality (5.6) follows now from (5.7). □

After these preparations we turn to the Schrödinger operator with bounded and compactly supported potential V. Now consider
$$(-\frac{d^2}{dx^2} + V - z)f = g \tag{5.9}$$
with $z \in \mathbb{C}$ with $\operatorname{Im} z \neq 0$ and V and g with compact support. Since $-\frac{d^2}{dx} + V$ is selfadjoint, the operator
$$(-\frac{d^2}{dx^2} + V - z)$$
is invertible.

We rewrite the equation (5.9) as (with $f = R_0(z)\tilde{f}$)
$$\tilde{f} + VR_0(z)\tilde{f} - g = 0 \tag{5.10}$$
and we want to study its solvability.

Suppose that $\tilde{f}$ satisfies (5.10) with $g = 0$:
$$\tilde{f} + VR_0(z)\tilde{f} = 0.$$
Then $F = R_0(z)\tilde{f}$ satisfies
$$-F'' + VF = zF. \tag{5.11}$$
If $\operatorname{Im} z \neq 0$, since V is compact supported, for $x > R$ we can write
$$F = c_+ e^{i\sqrt{z}x}$$
and for $x < -R$
$$F = c_- e^{-i\sqrt{z}x}.$$
We are particularly interested in the limit as $z \to \lambda$, $\lambda > 0$. In that case we have to pay attention whether we approach λ from above or below, which determines the behaviour of F outside $[-R, R]$.

Theorem 5.9. *Suppose that $g \in L^2(\mathbb{R}), V \in L^\infty(\mathbb{R})$ have compact support. Then Equation* (5.10) *has a unique solution for* $\operatorname{Im} z \neq 0$. *And for every $\lambda > 0$ the limit*

$$\lim_{z \to \lambda, \pm \operatorname{Im} z > 0} R(z) g$$

exists in C_b for $g \in L^2_{comp}$. We denote it by

$$R(\lambda \pm i0) g.$$

Then for all $R > 0$

$$\{g \in L^2, \operatorname{supp} g \subset [-R, R]\} \times \{z : \operatorname{Re} z > 0, \operatorname{Im} \pm z > 0\} \ni (g, z) \\ \mapsto R(z) g \in C_b([-R, R])$$

is continuous.

Proof. Suppose that

$$g \in L^2_R,\ V \in L^\infty_R, \quad L^p_R := \{h \in L^p : h \text{ is compactly supported in } (-R, R)\}.$$

The map

$$(g, z) \to (R_0(z) g)(x) = \frac{i}{2\sqrt{z}} \int_{-R}^{R} e^{i\sqrt{z}|x-y|} g(y) dy \in C^1_b(-R, R)$$

where $\sqrt{z}$ denotes the root with positive imaginary part is clearly continuous. $R_0(z)$ is compact as a map from L^2_R to $L^2(-R, R)$ and hence $V R_0(z)$ is also compact on L^2_R since $V : L^2(-R, R) \to L^2_R$ is continuous. Thus for $z = \lambda > 0$, (5.10) equals to search for $\tilde{f} \in L^2_R$ such that

$$(1 + K(\lambda \pm i0)) \tilde{f} = g \tag{5.12}$$

where $K = V R_0(\lambda \pm i0)$ is compact on L^2_R.

By the Fredholm alternative it is uniquely solvable provided there is only trivial solution to the homogenous problem with $g = 0$. It suffices to show that $F = R_0(\lambda \pm i0) \tilde{f} \in L^2_{loc}$ is zero (using that $R_0(\lambda \pm i0)$ is injective since $(-\partial_x^2 - \lambda) R_0(\lambda \pm i0) f = f$). Equivalently, we claim that the homogeneous problem

$$-F'' + VF = \lambda F, \tag{5.13}$$

with

$$F = c_\pm e^{i\sqrt{\lambda}|x|} \text{ for } |x| \geqslant R,$$

has only the trivial solution.

Suppose that F is a solution. We will prove that $c_\pm = 0$. Then 0 is the unique solution to (5.13) with

$$F(-R) = F'(-R) = 0.$$

Thus $\tilde{f} = 0$ if $g = 0$ in (5.12). Hence the operator on the lefthand side of (5.12) is invertible and we denote $R(\lambda \pm i0) = R_0(\lambda \pm i0)(1 + VR_0(\lambda \pm i0))^{-1}$. Since on $\{z : \mathrm{R}ez > 0, \mathrm{Im}\, z > 0\}$, $z \to VR_0(z)$ is continuous as map from L^2_R to L^2_R, the same is true for $z \to R(z)$ as map from L^2_R to $C_b([-R, R])$.

Take $F = R_0(\lambda + i0)\tilde{f}$ and hence $F = -R_0(\lambda + i0)VF$. By (5.6) with

$$\mathrm{Im} \int V|F|^2 dx = 0,$$

we have $F = -R_0(\lambda + i0)VF = -R_0(\lambda - i0)VF$. Hence by (5.5),

$$\lim_{r\to\infty} \frac{1}{2r} \int_{-r}^{r} |F|^2 dx = \lim_{r\to\infty} \frac{1}{2r} \int_{-r}^{r} R_0(\lambda + i0)VF\, \overline{R_0(\lambda - i0)VF} dx = 0,$$

and thus we get

$$\lim_{r\to\infty} \frac{1}{2r} \int_{r}^{r} |F|^2 dx = \frac{1}{2}(|c_+|^2 + |c_-|^2) = 0.$$

Thus F has compact support and it satisfies (5.13). It is the unique solution to the initial values problem with $F(-R) = F'(-R) = 0$, and hence it is trivial. We will see that this argument generalizes to higher dimensions. In one space dimension however there is also a more elementary argument.

Indeed, also $\bar{F}$ is a solution of (5.13) and the Wronskian

$$W = F'\bar{F} - F\bar{F}'$$

is constant:

$$W' = F''\bar{F} - F\bar{F}'' = (V - \lambda)F\bar{F} - F(V - \lambda)\bar{F} = 0.$$

We evaluate W at $x = R$ and $x = -R$ and obtain

$$|c_+|^2(2i\sqrt{\lambda}) = -|c_-|^2(2i\sqrt{\lambda})$$

which implies $c_\pm = 0$. $\square$

Definition 5.10 (Outgoing and incoming)**.** *We call f outgoing if it satisfies the Sommerfeld radiation condition*

$$f = c_\pm e^{i\sqrt{\lambda}|x|}$$

for $|x|$ large. We call it incoming if it satisfies the this condition with the opposite sign in the exponent.

It is interesting to note that $VR_0(z)f$ has an extension beyond the real axis with a pole at $z = 0$, which satisfies a generalized outgoing conditions where we continue the branch of $\sqrt{z}$ through λ.

The central definition is the distorted Fourier transform.

Definition 5.11 (Distorted Fourier transform)**.** *Suppose that f is compactly supported. We define its distorted Fourier transform by*

$$F_\pm f(k) = \mathcal{F}\Big[(1 + VR_0(k^2 \pm i0))^{-1} f\Big](k).$$

Let E^d be the closure of the span of eigenfunctions of $-\Delta + V$ and E^c its orthogonal complement. It is immediate that z is an eigenvalue iff one of the spectral measures carries a point mass. We define the projection to E^c by

$$P_c = \chi_{(0,\infty)}(-\Delta + V)$$

since there are no positive eigenvalues. For $d = 1$, 0 is not an eigenvalue neither.

Theorem 5.12. *For all $f \in L^2_{comp}$ we have*

$$\|P_c f\|_{L^2} = (2\pi)^{-\frac{1}{2}} \|F_\pm f\|_{L^2}. \tag{5.14}$$

Thus it extends to the unitary map from E^c to $L^2(\mathbb{R})$. Moreover

$$F_\pm e^{it(-\partial_{xx}+V)} = e^{it|k|^2} F_\pm.$$

Proof. Since

$$-\Delta + V - z = (-\Delta - z) + V,$$

by multiplying from the left and the right by $R_0(z)$ resp. $R(z)$

$$R_0(z) = R(z) + R_0(z)VR(z) = R(z) + R(z)VR_0(z),$$

we obtain $R(z) = R_0(z)(1 + VR_0(z))^{-1}$ and

$$R(\lambda \pm i0)f = R_0(\lambda \pm i0) f_{\lambda \pm i0}$$

using the notation

$$f_z = (1 + VR_0(z))^{-1} f.$$

Since

$$f = f_{\lambda \pm i0} + VR_0(\lambda \pm i0) f_{\lambda \pm i0}$$

and using again that the multiplication by V is symmetric to get

$$\langle R_0(\lambda + i0) f_{\lambda \pm i0}, f - f_{\lambda \pm i0} \rangle = \langle R_0(\lambda + i0) f_{\lambda \pm i0}, VR_0(\lambda \pm i0) f_{\lambda \pm i0} \rangle \in \mathbb{R}$$

and hence, using also (5.5),

$$\begin{aligned} \operatorname{Im}\langle R(\lambda \pm i0) f, f \rangle =& \operatorname{Im}\langle R_0(\lambda \pm i0) f_{\lambda \pm i0}, f \rangle \\ =& \operatorname{Im}\langle R_0(\lambda \pm i0) f_{\lambda \pm i0}, f_{\lambda \pm i0} \rangle \\ =& \frac{1}{4\sqrt{\lambda}} \Big(|\hat{f}_{\lambda \pm i0}(\sqrt{\lambda})|^2 + |\hat{f}_{\lambda \pm i0}(-\sqrt{\lambda})|^2 \Big). \end{aligned}$$

By Lemma 5.1, if f has compact support,

$$\begin{aligned} \|P_c f\|_{L^2}^2 =& \frac{1}{\pi} \int_0^\infty \operatorname{Im}\langle (-\Delta + V - \lambda - i0)^{-1} f, f \rangle d\lambda \\ =& \frac{1}{\pi} \int_0^\infty \frac{1}{4\sqrt{\lambda}} \Big(|\hat{f}_{\lambda \pm i0}(\sqrt{\lambda})|^2 + |\hat{f}_{\lambda \pm i0}(-\sqrt{\lambda})|^2 \Big) d\lambda \\ =& \frac{1}{2\pi} \int_{\mathbb{R}} |\hat{f}_{t^2 \pm i0}(t)|^2 dt \\ =& \frac{1}{2\pi} \|F_\pm f\|_{L^2}^2. \end{aligned}$$

This is a variant of Lemma 5.1: We have to apply it with a sequence of functions η_j converging to $\chi_{(0,\infty)}$. This implies identity (5.14). Next we prove

$$F_\pm(-\Delta - V) = m_{|k|^2} F_\pm$$

for f with compact support. Since

$$(-\Delta + V - \lambda) f = (-\Delta - \lambda) f + Vf$$

we have (taking limits)

$$(-\Delta + V - \lambda) f = (1 + VR_0(\lambda \pm i0))(-\Delta - \lambda) f$$

and hence

$$(1 + VR_0(\lambda \pm i0))^{-1} (-\Delta + V - \lambda) f = (-\Delta - \lambda) f.$$

We take a Fourier transform on both sides and evaluate at $\pm\sqrt{\lambda}$. The right hand side vanishes:

$$\mathcal{F}\Big[(-\Delta - \lambda)f\Big](\pm\sqrt{\lambda}) = 0$$

which implies the lefthand side also vanishes at $\pm\sqrt{\lambda}$:

$$\begin{aligned} 0 &= \mathcal{F}\big((1 + VR_0(k^2 \pm i0))^{-1}(-\Delta + V - k^2)f\big)(k)|_{k=\pm\sqrt{\lambda}} \\ &= F_\pm\Big[(-\Delta + V - k^2)f\Big](k)|_{k=\pm\sqrt{\lambda}}, \end{aligned} \tag{5.15}$$

hence

$$F_\pm(-\Delta + V)f(k) = k^2 F_\pm f(k)$$

for $f \in \mathcal{S}$. Now consider

$$g(t) = e^{-itk^2} F_\pm e^{it(-\Delta+V)} f$$

where $f \in D(-\Delta + V)$. Then

$$g' = e^{-itk^2} i(F_\pm(-\Delta + V) - k^2 F_\pm)e^{it(-\Delta+V)} f = 0.$$

We obtain the the isometry for smooth and compactly supported functions from Lemma 5.1. They are dense, and hence there is a unique extension to a unitary map. □

[12.07.2017]

[14.07.2017]

Theorem 5.13. $\mathrm{Ran}(W_\pm) = E^c$ *and*

$$F_\pm : E^c \to L^2$$

are unitary operators such that $F_\pm W_\pm$ is the Fourier transform. The scattering operator

$$S = W_+^* W_-$$

is a unitary operator on $L^2(\mathbb{R})$. It satisfies

$$h(-\Delta)S = Sh(-\Delta)$$

for any bounded measurable function h.

Proof. The range of $W_\pm$ is contained in E^c since $-\Delta$ has no eigenvalues. We claim

$$F_\pm \circ W_\pm = \mathcal{F}. \tag{5.16}$$

Let $f \in \mathcal{S}$. Then

$$W_- f = f - \int_{-\infty}^0 \frac{d}{dt} e^{it(-\Delta+V)} e^{it\Delta} f dt = f - \int_{-\infty}^0 e^{it(-\Delta+V)} iV e^{it\Delta} f dt.$$

Thus

$$F_- W_- f = F_- f - \lim_{\varepsilon \to 0} \int_{-\infty}^0 e^{\varepsilon t + it|k|^2} F_-(iVe^{it\Delta} f) dt$$

and

$$\begin{aligned} \lim_{\varepsilon \to 0} \int_{-\infty}^0 e^{\varepsilon t + it\lambda} F_-(iVe^{it\Delta} f) dt &= F_- V \lim_{\varepsilon \to 0} \int_{-\infty}^0 i e^{-it(-\Delta-\lambda+i\varepsilon)} f dt \\ &= -F_- V R_0(\lambda - i0) f \end{aligned}$$

hence

$$F_- W_- f(\pm\sqrt{\lambda}) = (F_-(1 + VR_0(\lambda - i0))f)(\pm\sqrt{\lambda}) = \mathcal{F} f(\pm\sqrt{\lambda}).$$

Using (5.16) we can easily complete the proof. The Fourier transform is surjective, hence also $F_\pm|_{E^c}$ is surjective. It is also injective, and thus $W_\pm$ is surjective. Then by definition

$$e^{it|k|^2} \mathcal{F} S \mathcal{F}^{-1} = e^{it|k|^2} F_+ W_+ W_+^* W_- W_-^* F_-^* = \mathcal{F} S \mathcal{F}^{-1} e^{it|k|^2},$$

and the last equality follows. □

In physics one usually uses the Fourier representation of S,

$$\mathcal{F} S \mathcal{F}^{-1} = F_+ F_-^{-1}.$$

Theorem 5.14. *For $\lambda > 0$ let*

$$u = u_\pm - R_0(\lambda \mp i0) V u$$

when

$$(-\Delta + V - \lambda) u = 0.$$

Then

$$\hat{u}_\pm = v_\pm^+ \delta_{\sqrt{\lambda}} + v_\pm^- \delta_{-\sqrt{\lambda}}.$$

The map (v_-^-, v_-^+) to (v_+^-, v_+^+) is denoted by $\Sigma(\lambda)$. Then

$$(\mathcal{F} S \mathcal{F}^{-1}) f|_{\{\pm\sqrt{\lambda}\}} = \Sigma(\lambda) f|_{\{\pm\sqrt{\lambda}\}}$$

and $\Sigma(\lambda)$ is unitary. It is called the scattering matrix at energy λ.

Proof. Since $(-\Delta - \lambda)R_0(\lambda \mp i0)Vu = Vu$, $(-\Delta - \lambda)u_\pm = 0$ and there exist $v_\pm^-, v_\pm^+$ such that

$$\hat{u}_\pm = v_\pm^- \delta_{-\sqrt{\lambda}} + v_\pm^+ \delta_{\sqrt{\lambda}}.$$

Now let

$$\hat{u}_+ = v_+^- \delta_{-\sqrt{\lambda}} + v_+^+ \delta_{\sqrt{\lambda}}.$$

We claim that

$$(1 + R_0(\lambda - i0)V)u = u_+$$

has a unique solution. This follows by the same argument as for $1 + VR_0(\lambda \pm i0)$ proven above. The same argument holds for the reverse sign and hence

$$u_+ = (1 + R_0(\lambda - i0)V)(1 + R_0(\lambda + i0)V)^{-1}u_-.$$

Hence $\Sigma(\lambda)$ is welldefined and bijective. It is an exercise to prove that it is unitary.

We write (with $d = 1$)

$$\begin{aligned}
&\langle F_+ f|_{\sqrt{\lambda}\mathbb{S}^{d-1}}, \Sigma(\lambda)\hat{u}_-|_{\sqrt{\lambda}\mathbb{S}^{d-1}}\rangle_{\sqrt{\lambda}\mathbb{S}^{d-1}} \\
&= \langle \mathcal{F}(1 + VR_0(\lambda + i0))^{-1} f|_{\sqrt{\lambda}\mathbb{S}^{d-1}}, \\
&\qquad \mathcal{F}(1 + R_0(\lambda - i0)V)(1 + R_0(\lambda + i0)V)^{-1}\mathcal{F}^{-1}\hat{u}_-\delta_{\sqrt{\lambda}\mathbb{S}^{d-1}}\rangle_{\sqrt{\lambda}\mathbb{S}^{d-1}} \\
&= \langle \mathcal{F}(1 + VR_0(\lambda - i0)V)^{-1} f|_{\sqrt{\lambda}\mathbb{S}^{d-1}}, \hat{u}_-\delta_{\sqrt{\lambda}\mathbb{S}^{d-1}}\rangle_{\sqrt{\lambda}\mathbb{S}^{d-1}} \\
&= \langle F_- f|_{\mathbb{S}_\lambda}, \hat{u}_-|_{\mathbb{S}_\lambda^{d-1}}\rangle
\end{aligned}$$

where we take the inner product with respect to $L^2(\sqrt{\lambda}\mathbb{S}^{d-1})$. Thus

$$F_+ f|_{\sqrt{\lambda}\mathbb{S}^{d-1}} = \Sigma(\lambda) F_- f|_{\sqrt{\lambda}\mathbb{S}^{d-1}}$$

for $f \in L^2_{comp}$.

□

We now turn to a more concrete representation. We consider solutions to

$$-u'' + Vu = \lambda u$$

with initial data

$$u(x) = e^{-i\sqrt{\lambda}x}$$

for $x \leqslant -R$ and V supported in $[-R, R]$. On the right it decomposes as

$$u(x) = a(\sqrt{\lambda} + i0)e^{-i\sqrt{\lambda}x} + b(\sqrt{\lambda} + i0)e^{i\sqrt{\lambda}x}, \quad x \geqslant R.$$

Since $u_\pm = v_\pm^- e^{-i\sqrt{\lambda}x} + v_\pm^+ e^{i\sqrt{\lambda}x} = (1 + R_0(\lambda \mp i0)V)u$, we derive from the above asymptotics of u at $|x| \geqslant R$ that

$$u_-(x) = ae^{-i\sqrt{\lambda}x}, \quad u_+(x) = e^{-i\sqrt{\lambda}x} + be^{i\sqrt{\lambda}x}.$$

Again the complex conjugate $\bar{u}$ is a solution, with the asymptotics

$$\bar{u} = e^{i\sqrt{\lambda}x} \text{ for } x \leqslant -R, \quad \bar{u} = \bar{a}e^{i\sqrt{\lambda}x} + \bar{b}e^{-i\sqrt{\lambda}x} \text{ for } x \geqslant R.$$

Thus

$$\Sigma(\lambda)\begin{pmatrix} a \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ b \end{pmatrix}$$

and

$$\Sigma(\lambda)\begin{pmatrix} \bar{b} \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ \bar{a} \end{pmatrix}.$$

The Wronskian $W = u\bar{u}' - u'\bar{u}$ is constant. On the left it is

$$W = \det\begin{pmatrix} u & \bar{u} \\ u' & \bar{u}' \end{pmatrix} = \det\begin{pmatrix} e^{-i\sqrt{\lambda}x} & e^{i\sqrt{\lambda}x} \\ -i\sqrt{\lambda}e^{-i\sqrt{\lambda}x} & i\sqrt{\lambda}e^{i\sqrt{\lambda}x} \end{pmatrix} = 2i\sqrt{\lambda},$$

and on the right it is

$$\det\begin{pmatrix} ae^{-i\sqrt{\lambda}x} + be^{i\sqrt{\lambda}x} & \bar{a}e^{i\sqrt{\lambda}x} + \bar{b}e^{-i\sqrt{\lambda}x} \\ -i\sqrt{\lambda}(ae^{-i\sqrt{\lambda}x} - be^{i\sqrt{\lambda}x}) & i\sqrt{\lambda}(\bar{a}e^{i\sqrt{\lambda}x} - \bar{b}e^{-i\sqrt{\lambda}x}) \end{pmatrix} = 2i\sqrt{\lambda}(|a|^2 - |b^2|).$$

Hence

$$|a|^2 = 1 + |b|^2.$$

We define the transmission coefficient T and the left/right coefficients L, R as follows:

$$T(\lambda + i0) = a(\lambda + i0)^{-1},$$
$$L(\lambda + i0) = a(\lambda + i0)^{-1}b(\lambda + i0), \quad R(\lambda + i0) = -a(\lambda + i0)^{-1}\bar{b}(\lambda + i0),$$

and hence

$$\Sigma(\lambda) = \begin{pmatrix} T(\lambda) & R(\lambda) \\ L(\lambda) & T(\lambda) \end{pmatrix}.$$

5.3 The case $d \geqslant 2$

This section serves as survey. The strategy is the same as for $d = 1$. There are no complete proofs in this section.

Let $d \geqslant 1$, $-\Delta : H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ and, for $\lambda \notin [0, \infty)$ we denote by $R_0(\lambda)$ the operator

$$(-\Delta - \lambda)^{-1} : L^2(\mathbb{R}^d) \to H^2(\mathbb{R}^d).$$

A Fourier transform translates $R_0(\lambda)$ to the multiplication operator

$$\phi \to (|k|^2 - \lambda)^{-1}\phi : L^2 \to L^2_{1+|k|^2}.$$

If $\lambda \in (0, \infty)$ then $(|k|^2 - \lambda)^{-1}$ is not locally integrable and hence not a distribution. This is the heart of the problem.

We define the space

$$B = \{f \in L^2 : \|f\|_{L^2(B_1(0))} + \sum_{j=0}^{\infty} 2^{j/2}\|f\|_{L^2(B_{2^j}(0)\setminus B_{2^{j-1}}(0))}\} < \infty$$

with the corresponding norm denoted by $\|\|_B$. We define

$$B^* = \{f \in L^2_{loc} : \max\{\|f\|_{L^2(B_1(0))}, \sup_j 2^{-j/2}\|f\|_{L^2(B_{2^j}(0)\setminus B_{2^{j-1}}(0))}\} < \infty\}.$$

Lemma 5.15. *B^* is the dual of B by the natural pairing.*

Lemma 5.16.

$$\int_{-\infty}^{\infty} \|u(x_1, \cdot)\|_{L^2} dx_1 \leqslant \sqrt{2}\|u\|_B$$

and

$$\|u\|_{B^*} \leqslant \sqrt{2} \sup_{x_1} \|u(x_1, \cdot)\|_{L^2}.$$

Theorem 5.17. *Let $\hat{u} = \hat{u}_0 d\mathbb{S}^{d-1}$. Then*

$$\|u\|_{B^*} \leqslant c\|\hat{u}_0\|_{L^2(\mathbb{S}^{d-1})}$$

The map $L^2(\mathbb{S}^{d-1}) \ni \hat{u}_0 \to u \in B^*$ is injective with closed range.

Proof. Since

$$u = (2\pi)^{-d/2} \int_{\mathbb{S}^{d-1}} e^{ix\cdot k}\hat{u}_0(k) dS(k)$$

we see that u is bounded in terms of $\|\hat{u}_0\|_{L^1(\mathbb{S}^{d-1})} \leqslant c\|u_0\|_{L^2(\mathbb{S}^{d-1})}$. By a partition of unity and rotation it suffices to consider

$$u(x) = \int_{B_1^{\mathbb{R}^{d-1}}} e^{ix\cdot(k'+h(k'))}\hat{u}_0(k') dk'$$

where $|\nabla h| \leqslant 1$ and estimate $\|u\|_{L^2(B_{2^j}\setminus B_{2^{j-1}})}$. $\square$

Theorem 5.18. *Let $M \subset \mathbb{R}^d$ be a C^1 hypersurface and $K \subset M$ a compact subset. Then*

$$\mathcal{S}(\mathbb{R}^d) \ni v \to v|_K \in L^2(K)$$

extends by continuity to a surjective map from B to $L^2(K)$.

Proof. If $\hat{u} = \hat{u}_0 dS$ then

$$|\langle \hat{u}_0, \hat{v}|_K \rangle_K| = |\langle u, v \rangle| \leqslant \|u\|_{B*} \|v\|_B$$

and the restriction of the Fourier transform is bounded. By Theorem 5.17 it is surjective since the adjoint is injective with closed range. □

If $z \notin [0, \infty)$ then z is in the resolvent set and there is a unique operator $R_0(z) : L^2 \to H^2$ which is a two sided inverse of $-\Delta - z$ and is given by the Fourier multiplier $(|k|^2 - z)^{-1}$.

Lemma 5.19. *$R_0(z)$ extends continuously to $[0, \infty)$ from both sides as a map from B to B^*. We denote it again by $R_0(\lambda \pm i0)$.*

Definition 5.20. *Let $\lambda > 0$. We call $u \in B^*$ λ outgoing /incoming if there exists $f \in B$ such that $u = R_0(\lambda \pm i0)f$.*

Lemma 5.21. *The following is equivalent.*

- *u is outgoing and incoming.*
- *u is in the closure of C_0^∞ in B^*.*
- *$\hat{f}(k) = 0$ for $|k|^2 = \lambda$.*

Let $V : \mathbb{R}^d \to \mathbb{R}$ be measurable. We will always assume that there exists $\varepsilon > 0$ and $C > 0$ such that

$$|V(x)| \leqslant C(1 + |x|)^{-1-\varepsilon}$$

We define

$$B_\Delta = \{u = v + \nabla w : v_j, w \in B\}$$

and

$$B_\Delta^* = \{f : \|f\|_B + \|\nabla f\|_B < \infty\}$$

Lemma 5.22. *V defines a compact multplication operator from ${B_\Delta}^*$ to B_Δ.*

We now continue as in the one dimensional case to define $R(z)$, extend it to $(0,\infty)$ from both sides, define the distorted Fourier transform by

$$F_\pm f(k) = \mathcal{F}[(1+VR_0(|k|^2 \pm i0))^{-1} f](k)$$

and the scattering operator S. Again one studies the scattering operator on the Fourier side, defines the unitary operators $\Sigma(\lambda) : L^2(\sqrt{\lambda}\mathbb{S}^{d-1}) \to L^2(\sqrt{\lambda}\mathbb{S}^{d-1})$.

One then studies solutions to

$$(-\Delta + V)(u + e^{ikx}) = \lambda(u + e^{ikx}), \quad \lambda = k^2,$$

which is equivalent to the Lippmann Schwinger equation.

$$-\Delta u + Vu = \lambda u - Ve^{ikx}.$$

At least formally

$$\Sigma(\delta_k) = \delta_k + \hat{u}|_{\sqrt{\lambda}\mathbb{S}^{d-1}}.$$

[14.07.2017]

[19.07.2017]

6 Symmetries, Groups and Spin

6.1 Quaternions, $SU(2)$ and $SO(3)$

Definition 6.1. *We fix a basis in $\mathbb{H} = \mathbb{R}^4$ which we denote by 1, i, j and k. We identify $\mathbb{R}^4$ with $\mathbb{C}^2$ with a basis 1, j by $i = i1$, $k = ij$. The multiplication is defined by*

$$i^2 = j^2 = k^2 = -1, ij = k, jk = i, ki = j, ji = -k, kj = -i, ik = -j$$

resp. by

$$(a + bj)(c + dj) = ac - b\bar{d} + (ad + b\bar{c})j.$$

The complex conjugate is given by

$$\overline{a + bj} = \bar{a} - bj.$$

We define real and imaginary part as for complex numbers

$$\operatorname{Re} x = \frac{1}{2}(x + \bar{x}), \quad \operatorname{Im} x = \frac{1}{2i}(x - \bar{x}).$$

The multiplication is associative but not commutative, and the distributive laws holds. We observe that

$$(a+bj)\overline{a+bj} = |a|^2 + |b|^2 + (-ab+ba)j = |a|^2 + |b|^2$$

and the inverse is given

$$(a+bj)^{-1} = \frac{1}{|a|^2+|b|^2}\overline{a+bj}.$$

With this multiplication $\mathbb{C}^2$ becomes a noncommutative field.

Lemma 6.2. *The sphere $\mathbb{S}^3$ becomes a group with this multiplication. Conjugation defines the inverse.*

A topological group is a group with a topology such that group multiplication is continuous. A (connected) Lie group is a connected topological group with a smooth structure. We will only consider groups of matrices which are a smooth submanifold in the space of matrices.

Definition 6.3. *Let G and H be (topological, smooth) groups. A map $\phi : G \to H$ is called a homomorphism if $\phi(1) = 1$ and $\phi(g_1g_2) = \phi(g_1)\phi(g_2)$ and if ϕ is continuous resp. smooth. It is called a (linear, continuous, smooth) representation if H is the group of invertible operators on a Hilbert space.*

Two representations $\gamma_V : G \to GL(V)$ and $\gamma_W : G \to GL(W)$ are called equivalent if there exists an invertible operator $T \in L(V,W)$ so that

$$\gamma_W(g)T = T\gamma_V(g), \quad \forall g \in G.$$

A representation is called unitary if $\gamma(g)$ is always unitary. An equivalence T is called unitary if the representations and T are unitary.

Lemma 6.4. *Every continuous finite dimensional representation of a finite dimensional Lie group is smooth.*

Proof omitted, similar to the smoothness of the exponential map.

Definition 6.5. *Let $d \geqslant 1$. We define*

$$GL(d,\mathbb{C}) = \{U \in \mathbb{C}^{d\times d} : \det U \neq 0\}$$

$$SL(d,\mathbb{C}) = \{U \in \mathbb{C}^{d\times d} : \det U = 1\}$$

$$U(d,\mathbb{C}) = \{U \in \mathbb{C}^{d\times d} : U^*U = 1\}$$

$$SU(d) = \{U \in \mathbb{C}^{d\times d} : U^*U = 1, \det(U) = 1\}$$

and

$$GL(d,\mathbb{R}) = \{O \in \mathbb{R}^{d\times d} : \det(O) \neq 0\}$$
$$SL(d,\mathbb{R}) = \{O \in \mathbb{R}^{d\times d} : \det(O) = 1\}$$
$$O(d) = \{O \in \mathbb{R}^{d\times d} : O^T O = 1\}$$
$$SO(d) = \{O \in \mathbb{R}^{d\times d} : O^T O = 1, \det(O) = 1\}$$

which are smooth groups with the matrix multiplication. More generally we define the corresponding groups ($GL(H)$) for Hilbert spaces. If G is a group then a homomorphism $\phi : G \to GL(H)$ is called a representation.

The group $\mathbb{S}^3$ acts in three different ways on $\mathbb{R}^4$:

1. $(g,x) \to gx$
2. $(g,x) \to xg^{-1}$
3. $(g,x) \to gxg^{-1}$.

Only the second one gives an action of $SU(2)$.

The last action commutes with conjugation and taking real parts

$$\operatorname{Re} gxg^{-1} = \frac{1}{2}(gxg^{-1} + \bar{g}^{-1}\bar{x}\bar{g}) = g\frac{1}{2}(x+\bar{x})g^{-1}$$

As a consequence $\mathbb{S}^3$ acts on $\mathbb{R}^3$ which we identity with the quaternians with real part 0.

Lemma 6.6. *The group $\mathbb{S}^3$ acts on $\mathbb{C}^2$ by*

$$\gamma_1 : \mathbb{S}^3 \times \mathbb{C}^2 \ni (g,z) \to zg^{-1} \in \mathbb{C}^2$$

In coordinate

$$\mathbb{S}^3 \ni (a+bj) \to \begin{pmatrix} \bar{a} & -b \\ \bar{b} & a \end{pmatrix} \in SU(2).$$

It is an isomorphic homomorphism.

The map

$$\gamma_2 : \mathbb{S}^3 \times \mathbb{R}^3 \ni (g, x_1 i + x_2 j + x_3 k) \to g(x_1 i + x_2 j + x_3 k)g^{-1}$$

can be written in coordinates as

$$\mathbb{S}^3 \ni (a+bi+cj+dk) \to \begin{pmatrix} a^2+b^2-c^2-d^2 & 2(ad+bc) & 2(-ac+bd) \\ -2(ad-cb) & a^2-b^2+c^2-d^2 & 2(ab+cd) \\ 2(ac+bd) & 2(cd-ab) & a^2-b^2-c^2+d^2 \end{pmatrix} \in SO(3)$$

is surjective and it maps two points g_1, g_2 to the same matrix iff $g_1 = -g_2$.

Proof. We want to determine the matrix corresponding to $\gamma_1(a+bj)$. We check

$$1(a+bj)^{-1} = \bar{a} - bj$$

and

$$j(a+bj)^{-1} = j(\bar{a}-bj) = aj + \bar{b}.$$

It is not hard to see that this matrix is in $SU(2)$, and that every element in $SU(2)$ can be represented in this fashion.

Let us work out the map $\gamma_2 : \mathbb{S}^3 \to SO(3)$. Let $a^2+b^2+c^2+d^2 = 1$. Then

$$\begin{aligned}(a-bi-cj-dk)i(a+bi+cj+dk) =& (ai+b+ck-dj)(a+bi+cj+dk)\\ =& (a^2+b^2-c^2-d^2)i + 2(cb-ad)j + 2(ac+bd)k\end{aligned}$$

$$\begin{aligned}(a-bi-cj-dk)j(a+bi+cj+dk) =& (aj-bk+c+di)(a+bi+cj+dk)\\ =& 2(ad+bc)i + (a^2-b^2+c^2-d^2)j + 2(cd-ab)k\end{aligned}$$

$$\begin{aligned}(a-bi-cj-dk)k(a+bi+cj+dk) =& (ak+bj-ci+d)(a+bi+cj+dk)\\ =& 2(-ac+bd)i + 2(ab+cd)j + (a^2-b^2-c^2+d^2)k\end{aligned}$$

It is immediate that these maps are homomorphisms. For $SO(3)$ it is immediate that g_1 and g_2 are mapped to the same point if they are antipodal points. An element of $SO(3)$ is a rigid rotation and determined by an angle and an oriented axis of rotation. The axis of rotation is given by the eigenvector to the eigenvalue 1. Since

$$(1+\operatorname{Im} x)^{-1}\operatorname{Im} x(1+\operatorname{Im} x) = (1+\operatorname{Im} x)^{-1}(1+\operatorname{Im} x)(1+\operatorname{Im} x) - 1 = \operatorname{Im} x$$

it is given by the imaginary part. To determine the angle of rotation we restrict to consider the action $a+ib$ on j. Then

$$(a-ib)j(a+ib) = (a-ib)(aj-bk) = (a^2-b^2)j - 2abk$$

which is equal to j if and only if $a = \pm 1$. It follows that $\gamma_2(g) = \gamma_2(h)$ implies $g = \pm h$. It is an exercise to deduce surjectivity. □

Examples of representations.

1. $SU(d)$ acts on $\mathbb{C}^d$ in the natural fashion. Similarly $SO(d)$ acts on $\mathbb{R}^d$.

2. $SU(d)$ acts on the space of homogeneous complex polynomials of degree m. Similarly $SO(d)$ acts $\mathbb{R}^d$ and on the space of harmonic polynomials of degree m on $\mathbb{R}^d$.

3. Lie groups act on the tangent space at 1.

The case $SU(1)$. The group $SU(1)$ has dimension 1 and is isomorphic to the rotations of the complex plane C.

There is an isomorphism $SU(1) \to SO(2)$. $SO(2)$ is the group of roations of the real two dimensional plane.

Let $m \geqslant 0$. Then $SU(2)$ acts on the space W_m of complex homogeneous polynomials of degree m in two variables. A simple counting argument shows that the dimension of W_m is $m+1$.

$SO(3)$ acts on the space V_m of harmonic polynomials of degree m. Its dimension is $1+2m$.

Definition 6.7. *The Hopf map $\mathbb{S}^3 \to \mathbb{S}^2$ defined by*

$$H : (a+bj) \to (2a\bar{b}, |a|^2 - |b|^2)$$

maps x and y to the same point iff there exists $\gamma \in \mathbb{C}$, $|\gamma| = 1$ with $y = \gamma x$.

It should be possible to relate the represention of $SO(3)$ on V_m and the representation of $SU(2)$ on W_{2m} via the Hopf map, but I did not manage to do that.

[19.07.2017]

[21.07.2017]

6.2 Decomposition into irreducible representations

Definition 6.8. *A representation $\gamma : G \mapsto GL(V)$ is called irreducible if there is no nontrivial invariant subspace of V.*

We consider compact topological groups G with a probability measure μ which is invariant under the group action. It is called Haar measure. This is certainly true for every compact Lie group, and in particular for $\mathbb{S}^3 = SU(2)$ and $SO(3)$.

Lemma 6.9. *Let $\gamma : G \to GL(\mathbb{C}^d)$. Then there exists a Hermitian inner product so that γ is unitary.*

Proof. Let $(.,.)$ be any Hermitian inner product on $\mathbb{C}^d$. We define

$$\langle u, v\rangle = \int_G (\gamma(g)u, \gamma(g)v) d\mu(g).$$

Then $\langle \gamma(g)u, \gamma(g)v\rangle = \langle u, v\rangle$ for all u, v and g. □

Lemma 6.10 (Schur)**.** *If γ and γ' are irreducible representations on V resp V' and if $T \in L(V, V')$ satisfies $T\gamma(g) = \gamma'(g)T$ for all g then either T is bijective or $T = 0$.*

Proof. Both the null space and the range of T are invariant subspaces, and then these are the only possibilities. $\square$

Lemma 6.11 (Schur 2)**.** *If in the previous lemma $V = V'$ then T is a multiple of the identity.*

Proof. Every geometric eigenspace is invariant, and hence either $\{0\}$ or V since the representation is irreducible. $\square$

Lemma 6.12. *Let γ and γ' be irreducible unitary representations on the finite dimensional complex vector spaces V resp. V'. Let $v, w \in V$ and $v', w' \in V'$. If*

$$\int_G \overline{\langle \gamma(g)v, w\rangle_V} \langle \gamma'(g)v', w'\rangle_{V'} d\mu(g) \neq 0$$

then there exists $L \in L(V, V')$ invertible such that

$$\gamma'(g)L = L\gamma(g) \qquad \text{for all } g.$$

If $\gamma = \gamma'$ then

$$\int_G \overline{\langle \gamma(g)v, w\rangle} \langle \gamma(g)v', w'\rangle d\mu(g) = (\dim V)^{-1} \overline{\langle v, v'\rangle} \langle w, w'\rangle. \tag{6.1}$$

Proof. Let $l \in L(V, V')$ and

$$L = \int_G \gamma'(g) l \gamma(g^{-1}) d\mu(g).$$

Then

$$\gamma'(g)L = L\gamma(g)$$

and hence L is either trivial or invertible. The second happens if the integral is not zero: Choose $l(w) = \langle w, v\rangle v'$, then

$$\begin{aligned}\int_G \overline{\langle \gamma(g)v, w\rangle_V} \langle \gamma'(g)v', w'\rangle_{V'} d\mu(g) &= \int_G \langle \gamma(g^{-1})w, v\rangle_V \langle v', \gamma'(g^{-1})w'\rangle_{V'} d\mu(g) \\ &= \int_G \langle l\gamma(g^{-1})w, \gamma'(g^{-1})w'\rangle_{V'} d\mu(g) = \langle Lw, w'\rangle_{V'}.\end{aligned}$$

If $\gamma = \gamma'$ we argue in the same fashion. Then $L = \lambda 1$ and

$$\begin{aligned}\lambda \dim V &= \operatorname{tr} L \\ &= \int_G \operatorname{tr} \gamma(g) l \gamma(g)^{-1} d\mu(g) \\ &= \int_G \operatorname{tr} l d\mu(g) = \operatorname{tr} l.\end{aligned}$$

Thus

$$\int_G \overline{\langle \gamma(g)v, w\rangle} \langle \gamma'(g)v', w'\rangle d\mu(g) = \langle Lw, w'\rangle = \lambda \langle w, w'\rangle = \frac{\operatorname{tr} l}{\dim V} \langle w, w'\rangle,$$

where we choose $l(w) = \langle w, v\rangle v'$ so that $\operatorname{tr} l = \overline{\langle v, v'\rangle}$. The formula (6.1) follows. □

Theorem 6.13. *Let H be a separable complex vector space and $\gamma : G \to GL(H)$ a unitary representation. Then there exists at most countably many closed finite dimensional invariant subspaces H_j whose closure span H such that $\gamma|_{H_j}$ is irreducible.*

Proof. We just prove the statement for finite dimensional H. To see that there is irreducible representation on a subspace we pick an invariant subspace of minimal dimension. It carries a representation which is necessarely irreducible. The orthogonal complement is invariant and we construct the subspaces recursively. □

6.3 The Lie algebra of matrix groups

As a vector space a Lie algebra is the tangent space of a Lie group at 1. The matrix multiplication turns the tangent space into a Lie algebra.

(The materials given here are classical theory for Lie algebra and can be found in various classic references, e.g. Kristopher Tapp "Matrix Groups for Undergraduates")

Lemma 6.14 (Lie algebra). *1. The tangent space $gl(d;\mathbb{C})$ of $GL(d;\mathbb{C})$ at the identity is $\mathbb{C}^{d\times d}$. The tangent space $sl(d;\mathbb{C})$ of $SL(d;\mathbb{C})$ consists of all matrices with trace 0. The tangent space $u(d)$ of $U(d)$ consists of all matrices $A \in \mathbb{C}^{d\times d}$ with*

$$A^* = -A.$$

The tangent space $su(d)$ is the intersection $sl(d;\mathbb{C}) \cap u(d)$.

2. *The tangent space* $gl(d;\mathbb{R})$ *of* $GL(d;\mathbb{R})$ *at the identity is* $\mathbb{R}^{d\times d}$. *The tangent space* $sl(d;\mathbb{R})$ *of* $SL(d;\mathbb{R})$ *consists of all matrices with trace* 0. *The tangent space* $o(d)$ *of* $O(d)$ *consists of all matrices* $A \in \mathbb{C}^{d\times d}$ *with*

$$A^T = -A.$$

The tangent space $so(d)$ *is the intersection* $sl(d;\mathbb{R}) \cap o(d)$.

3. *The Lie product is defined by*

$$[A, B] = AB - BA.$$

It satisfies Jacobi identity

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0,$$

and the trace form

$$\operatorname{tr}([A, B]C) = \operatorname{tr}(B[A, C]).$$

4. *The matrix exponential* exp *defines a map from the Lie algebra to the group such that*

$$\begin{gathered}
\exp(0) = 1 \\
\frac{d}{dt}\exp(tA) = A\exp(tA) = \exp(tA)A \\
\frac{\partial^2}{\partial s\partial t}\exp(sA)\exp(tB)\exp(-sA)\exp(-tB)\Big|_{s=t=0} = AB - BA = [A, B] \\
\exp(A)^* = \exp(A^*)
\end{gathered} \tag{6.2}$$

The matrix exponential maps a neighborhood of 0 *of the Lie algebra to a neighbirhood of* 1 *of the group.*

5. *If* H, G *are finite dimensional smooth matrix groups, if* $\phi : G \to H$ *is a smooth homomorphism then* $d\phi(1)$ *maps the tangent space at* 1 *in* G *to the tangent space at* 1 *in* H. *It is an algebra homomorphism of the Lie algebras. In particular*

$$[\phi(A), \phi(B)] = \phi([A, B]). \tag{6.3}$$

6. *The matrix exponentials* $\exp : su(d) \to SU(d)$ *and* $\exp : so(d) \to SO(d)$ *are surjective.*

Proof. The group $GL(d,\mathbb{C})$ is defined as $\{U : \det U \neq 0\}$. The map to the determinant is smooth and nondegenerate: The rank $D \det U$ is always 1 since

$$\frac{d}{dt} \det e^{it} A = \det(A) \frac{d}{dt} e^{idt}.$$

Hence for any $A \in \mathbb{C}^{d\times d}$, there exists ϵ such that $\det(1 + tA) \neq 0$ for $|t| < \epsilon$. $A \in gl(d,\mathbb{C})$.

Since if $\gamma : (-\epsilon, \epsilon) \to SL(d;\mathbb{C})$ differentiable with $\gamma(0) = 1$, $\gamma'(0) = A$, $\det(\gamma(t)) = 1$, then $\gamma(t) = 1 + tA + O(t^2)$ and

$$\det(1 + tA) = 1 + t \operatorname{tr} A + O(t^2) = \det(\gamma(t)) + O(t^2) = 1 + O(t^2),$$

the tangent space $sl(d;\mathbb{C})$ consists of all matrices with trace 0. Similarly $U(d)$ is defined by

$$U^*U = 1.$$

The derivative of $U \to U^*U$ at $U = 1$ is

$$A \to A^* + A$$

and the tangent space is $\{A : A^* + A = 0\}$. The other relations are similar.

We verify the Jacobi identity for matrices:

$$A(BC-CB)-(BC-CB)A+B(CA-AC)-(CA-AC)B+C(AB-BA)-(AB-BA)C = 0.$$

Also the calculation for the trace form is easy:

$$\operatorname{tr}[ABC - BAC - BAC + BCA] = \operatorname{tr}[A(BC) - (BC)A] = 0.$$

The formulas for the matrix exponential follow from the definition. We want to verify that the matrix exponential of an element of the Lie algebra is an element of the Lie group. Since the Lie algebra is the tangent space at 1, we see that

$$\operatorname{dist}(\exp(ta), G) \leqslant C|t|^2.$$

Since

$$\exp(a) = \prod_{j=1}^{m} \exp(\frac{1}{m}a),$$

let g be the closest element in G to $\exp(\frac{1}{m}a)$. Then, with $h = \exp(\frac{1}{m}a)$

$$\operatorname{dist}(\exp(a), G) \leqslant \operatorname{dist}(h^m, g^m) \leqslant \sum_{j=0}^{m-1} \|h^j(h-g)g^{m-1-j}\| \leqslant Cm/m^2 \to 0 \text{ as } m \to \infty.$$

The statement about diffeomorphism of neighborhoods of 0 resp 1 is a consequence of the implicit or inverse function theorem with local coordinates which we skip.

Formula (6.3) follows from (6.2) and the surjectivity of the matrix exponential restricted to a neighborhood of 0 to a neighborhood of 1 which we can interprete as a parmetrization of a neighborhood of 1.

We turn to surjectivity of the matrix exponential for $SU(d)$ and $SO(d)$. Let $U \in SU(d)$. It is normal and hence it suffices to consider a diagonal matrix with diagonal entries of modulus 1,

$$U = \begin{pmatrix} e^{i\lambda_1} & 0 & \dots & 0 \\ 0 & e^{i\lambda_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & e^{i\lambda_d} \end{pmatrix} = \exp \begin{pmatrix} i\lambda_1 & 0 & \dots & 0 \\ 0 & i\lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & i\lambda_d \end{pmatrix}.$$

The case of $SO(d)$ is a bit more involved, but it is easy in $d = 3$ since elements of $SO(3)$ are rotations around an axis. □

Definition 6.15. *A finite dimensional representation of a Lie algebra g is an algebra homomorphism from g to $gl(\mathbb{C}^d)$. It is called irreducible if there is no nontrivial invariant subspace.*

The derivative of a representation at the identity is a homomorphism of the Lie algebras. In particular the derivative of a representation at 1 is representation of the Lie algebra. It is irreducible if and only if the representation of the group is irreducible.

[21.07.2017]

[25.07.2017]

6.4 Irreducible representations of $SU(2)$ and $SO(3)$

Consider an irreducible representation ρ of $SU(2) \subset SL(2;\mathbb{C})$ on $\mathbb{C}^2$. The derivative defines a representation $D\rho : su(2) \to \mathbb{C}^{2\times 2}$. It is again irreducible. The space $su(2)$ has dimension three and $D\rho$ is uniquely described by giving the image of i times the Pauli matrices

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}.$$

The Lie algebra $sl(2;\mathbb{C})$ of $SL(2;\mathbb{C})$ has complex dimension 3 and a complex basis given by the Pauli matrices. Thus it is the complexification of $su(2)$ and every complex representation of ρ determines a representation of $sl(2;\mathbb{C})$. This representation is irreducible since already the restriction to $su(2)$ is irreducible. Vice versa: If we start with an irreducible complex representation of $sl(2;\mathbb{C})$ it restriction to $su(2)$ is irreducible. The exponential defines an irreducible representation of $SU(2)$.

Any equivalence of representations of $SU(2)$ leads to an equivalence of representations of $sl(2;\mathbb{C})$.

Theorem 6.16. *The representations $\rho_m : SU(2) \to L(W_m)$ are irreducible. Every irreducible representation is equivalent to one of the ρ_m.*

Proof. We consider finite dimensional representations γ of $sl(2;\mathbb{C})$. We choose the basis

$$H = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad E = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad F = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Then

$$[H, E] = 2E, \quad [H, F] = -2F \quad [E, F] = H.$$

The derivative of γ at the identity is a representation ρ of the Lie algebra $\rho([H, E]) = [\rho(H), \rho(E)]$. Let $\rho : sl(2;\mathbb{C}) \to L(V)$ be an irreducible representation of this Lie algebra. We pick an eigenvector v of $\rho(H)$ with eigenvalue λ. Then

$$\rho(H)\rho(E)v = [\rho(H), \rho(E)]v + \rho(E)\rho(H)v = (\lambda + 2)\rho(E)v.$$

$$\rho(H)\rho(F)v = [\rho(H), \rho(F)]v + \rho(F)\rho(H)v = (\lambda - 2)\rho(F)v.$$

Let $\rho(F)^{j+1}$ be the smallest power so that $\rho(F)^{j+1}v = 0$. Such a j exists since all nonzero vectors $\rho(F)^j v$ are eigenvectors to different eigenvalues, and hence linearly independent. We recall that $\dim V < \infty$. Let $v_0 = \rho(F)^j v$. It is an eigenfunction of $\rho(H)$ to the eigenvalue λ_0. Let $v_j = \rho(E)^j v_0$ and let $N + 1$ be the first power so that $\rho(E)^{N+1} v_0 = 0$. Then $\{v_j\}$ span an invariant subspace, and, since the representation is irreducible this subspace is the full space. Moreover

$$\sum_{j=0}^{N} (\lambda_0 + 2j) = \operatorname{tr} \rho(H) = \operatorname{tr} \rho([E, F]) = \operatorname{tr}(\rho(E)\rho(F) - \rho(F)\rho(E)) = 0,$$

that is, $\lambda_0(N + 1) + N(N + 1) = 0$ and hence $\lambda_0 = -N$. So for every $N \geqslant 0$ there is at most one irreducible representation of $su(2)$ dimension $N + 1$ with $\lambda_0 = -N$ up to homomorphism. Let γ_j be irreducible unitary representations of $SU(2)$ on the $\mathbb{C}^N$, $j = 1, 2$. Then the representations

$\rho_j = D\gamma_j(1)$ are irreducible representations of $su(2)$, which are unitarily equivalent by the first part of the proof. Exponentiation shows that then γ_1 and γ_2 are equivalent.

It remains to check that the representations γ_m on the harmonic polynomials of degree m are irreducible. We have

$$\gamma \begin{pmatrix} z^{-1} & 0 \\ 0 & z \end{pmatrix} z_1^j z_2^{m-j} = z^{m-2j} z_1^j z_2^{m-j}$$

and

$$\gamma \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix} z_1^j z_2^{m-j} = (z_1 + t z_2)^j z_2^{m-j}$$

hence

$$\rho(H) z_1^j z_2^{m-j} = (m-2j) z_1^j z_2^{m-j}$$

and

$$\rho(E) z_1^j z_2^{m-j} = j z_1^{j-1} z_2^{m+1-j}$$
$$\rho(F) z_1^j z_2^{m-j} = (m-j) z_1^{j+1} z_2^{m-1-j}$$

Thus $\rho(E)^j z_1^m$ is a basis of W_m and the representation is irreducible. □

Theorem 6.17. *The representation $\gamma_m : SO(3) \to GL(V_m)$ are irreducible. Every irreducible representation is equivalent to one of them.*

Proof. Let $\gamma : SO(3) \to O(d)$ be a irreducible representation of $SO(3)$. It defines a unitary representation on $\mathbb{C}^d$ by a diagonal action on real and imaginary part. The canonical map $\gamma_0 : SU(2) \to SO(3)$ induces an isomorphism of the Lie algebras, and then a representation of $sl(2, \mathbb{C})$ as above, which is irreducible. Thus the associated representation of $SU(2)$ is irreducible and $-1 \in SU(2)$ is mapped to $1 \in SO(3)$ and thus d has to be odd. Tracing these maps shows that irreducible representations of the same dimension are equivalent.

It is a little harder than for $SU(2)$ to check that the representation γ_m are irreducible. □

The number $(d-1)/2 = m/2$ is called the spin.

6.5 The spin

We begin with considering the symmetries of a single particle Hilbert space. I did not find these considerations explicitly in the physics literature, but I describe what seems to be the essence of the considerations in the physics literature leading to single and multi particle Hilbert spaces.

6.5.1 What is a single particle Hilbert space?

1. The Heisenberg commutation relations $[i\partial_j, x_k] = i\delta_{jk}$ are central. We have seen that a rigorous formulation consists in asking that the Heisenberg group acts unitarily on the Hilbert space such that $(0, 0, t)$ is mapped to the multiplication by $e^{i\hbar t}$ (with $\hbar = 1$ without loss of generality). By the Stone-von Neumann theorem we know all such irreducible representations.

2. The Euclidean space $\mathbb{R}^3$ is invariant under rigid rotations resp. the action of $SO(3)$, and hence also of $SU(2)$. Every element of $GL(d)$ defines automorphism of $\mathcal{H}^d$:
$$g : (x, k, t) \to (gx, g^{-T}k, t).$$
In particular we obtain an action of $g \in SU(2)$ on $\mathcal{H}^3$. This defines a homomorphism from $SU(2)$ into the automorphisms of $\mathcal{H}^3$.

3. This actions allows to define a semidirect product of $G \otimes_\gamma H$ which makes $G \times H$ group by
$$(g_1, h_1) * (g_2, h_2) \to (g_1 g_2, h_1 \gamma(g_1) h_2).$$
It is not difficult to check that this defines a group.

4. A single particle Hilbert space is an irreducible unitary representation of $SU(2) \otimes_\gamma \mathcal{H}^3$ satisfying the Heisenberg commutation relations.

5. Up to equivalence the irreducible representations are given by $H = L^2(\mathbb{R}^3; \mathbb{C}^d)$ with
$$\gamma(g)\psi(x) = \gamma_d \psi(\gamma_0(g)x)$$
where $\gamma_0 : SU(2) \to SO(3)$.

6.5.2 What is a multiparticle Hilbert space?

A multiparticle Hilbert space is the direct product of the corresponding single particle Hilbert space. For two particle
$$L^2(\mathbb{R}^3; \mathbb{C}^{d_1}) \otimes L^2(\mathbb{R}^3; \mathbb{C}^{d_2}) = L^2(\mathbb{R}^6; \mathbb{C}^{d_1 \times d_2}).$$
The representation of $SU(2)$ on $\mathbb{C}^{d_1 \times d_2}$ is reducible in general!

6.5.3 What is the Hilbert space for identical particles?

For identical particles exchanging identical particles (which means the action of the symmetry group $\psi(x_1, j_1, x_2, j_2) \to \psi(x_2, j_2, x_1, j_1)$ where j_k describes the spin variable) leads to a multiplication by $e^{i\gamma}$ for some $\gamma \in \mathbb{R}$. It is not hard to see that γ does not depend on ψ, and, since replacing twice we get the identity we have $e^{i\gamma} = \pm 1$.

Theorem 6.18 (Spin-statistic)**.** *If $d/2 \notin \mathbb{Z}$ we have $e^{i\gamma} = -1$ and particles are called Fermions. If $d/2 \in \mathbb{Z}$ we have $e^{i\gamma} = 1$ and particles are called Bosons.*

According to Weinberg this theorem can only be proven for field theory. It seems to me however that the arguments in field theory directly work in our setting here.

Electrons, protons and neutrons have spin 1/2, photon have spin 1.

Fermions satisfy the Pauli exclusion principle: Two electrons cannot be in the same state since exchanging them would not change the wave function, but, being Fermions, it has to -1 times the wave function.

Now we would have to go back and discuss the hydrogen atom, other atoms, electrons in an electric and magnetic field, allowing interaction with the spin, modify the Hamiltonians for atoms to allow for interaction of the spin, discuss larger atoms and also the nucleus.

Next one should discuss the interaction of atoms with light and statistical physics of quantum systems leading to describing black body radiation.

A Appendix

A.1 Gaussian integrals

The theorem of Fubini: Suppose that f is integrable on $\mathbb{R}^{n_1+n_2}$. Then $x_2 \to f(x_1, x_2)$ is integrable for almost every x_1, $x_1 \to \int f(x_1, x_2) d\mathcal{L}^{n_2}$ is integrable, and

$$\int_{\mathbb{R}^{n_1}} \int_{\mathbb{R}^{n_2}} f(x_1, x_2) d\mathcal{L}^{n_2}(x_2) d\mathcal{L}^{n_1}(x_1) = \int_{\mathbb{R}^n} f(x_1, x_2) d\mathcal{L}^{n_1+n_2}(x_1, x_2).$$

We use this to evaluate certain integrals and to determine the volume of the unit ball, with $d\mathcal{L}^n$ the Lebesgue measure. First

$$\begin{aligned} \int_{\mathbb{R}^n} e^{-|x|^2} d\mathcal{L}^n(x) &= \int_{\mathbb{R}^{n_1}} e^{-|x_1|^2} \int_{\mathbb{R}^{n_2}} e^{-|x_2|^2} d\mathcal{L}^{n_2}(x_2) d\mathcal{L}^{n_1}(x_1) \\ &= \int_{\mathbb{R}^{n_1}} e^{-|x_1|^2} d\mathcal{L}^{n_1}(x_1) \int_{\mathbb{R}^{n_2}} e^{-|x_2|^2} d\mathcal{L}^{n_2}(x_2) \end{aligned}$$

and the integral over the Gaussian in $\mathbb{R}^{n_1+n_2}$ is the product of the integrals of Gaussians in $\mathbb{R}^{n_1}$ and $\mathbb{R}^{n_2}$. Recursively we see that the integral over the Gaussian in $\mathbb{R}^n$ is the nth power of the one dimensional integral over the Gaussian. We can also use the theorem of Fubini in a different fashion:

$$\begin{aligned}\int_{\mathbb{R}^n} e^{-|x|^2} d\mathcal{L}^n(x) =&\mathcal{L}^{n+1}(\{(x,t) : 0 \leqslant t \leqslant e^{-|x|^2}\})\\ =&\int_0^\infty \mathcal{L}^n(\{x : e^{-|x|^2} > t\})dt = \int_0^1 \mathcal{L}^n(B_{(-\ln t)^{\frac{1}{2}}}(0))dt\\ =&\mathcal{L}^n(B_1(0))\int_0^1 (-\ln t)^{\frac{n}{2}} dt\\ =&\mathcal{L}^n(B_1(0))\int_0^\infty s^{\frac{n}{2}} e^{-s} ds\\ =&\mathcal{L}^n(B_1(0))\Gamma(\frac{n+2}{2})\end{aligned}$$

where Γ is the Gamma function. Hence

$$\int_{\mathbb{R}^2} e^{-|x|^2} dx = \pi, \qquad \int_{\mathbb{R}} e^{-|x|^2} dx = \sqrt{\pi}, \qquad \int_{\mathbb{R}^n} e^{-|x|^2} dx = \pi^{\frac{n}{2}},$$

$$\Gamma(1/2) = 2\Gamma(3/2) = \sqrt{\pi}$$

and

$$\mathcal{L}^n(B_1(0)) = \frac{\pi^{n/2}}{\Gamma((n+2)/2)}.$$

A.2 Holomorphic functions

Definition A.1. *Let $U \subset \mathbb{C} = \mathbb{R}^2$ be open. We call $f : U \to \mathbb{C}$ holomorphic if it is differentiable at every point, or if the Jacobi matrix is a multiple of a rotation at every point.*

A 2×2 matrix is a multiple of a rotation iff is has the form

$$\begin{pmatrix} a & b \\ -b & a \end{pmatrix} = \sqrt{a^2+b^2} \begin{pmatrix} \frac{a}{\sqrt{a^2+b^2}} & \frac{b}{\sqrt{a^2+b^2}} \\ \frac{-b}{\sqrt{a^2+b^2}} & \frac{a}{\sqrt{a^2+b^2}} \end{pmatrix}.$$

This is equivalent to the existence of the limit

$$\lim_{z \to z_0} \frac{f(z) - f(z_0)}{z - z_0} \in \mathbb{C}$$

which the definition of complex differentiability.

Theorem A.2. *Holomorphic functions are analytic. Their complex Taylor series converge in a neighborhood of every points.*

Let γ be an oriented piecewise C^1 curve in U and assume that f is holomorphic in U. Then we define the complex line integral by

$$\int_\gamma f(z)dz = \int_a^b f(\gamma(t))\gamma'(t)dt$$

for a parametrization of γ. The result is independent of γ.

Theorem A.3 (Cauchy integral theorem)**.** *Suppose that U is simply connected and γ is closed. Then*

$$\int_\gamma f(z)dz = 0$$

Sketch of the proof: Assuming that $f \in C^1$ one obtains the claim by an application of the divergence theorem.

We also need a simple version of the residue theorem. Let $V \subset \bar{V} \subset U$ be open so that $\bar{V}$ is compact, with a piecewise C^1 boundary. Then there is a unique path γ which runs around V so that V always lies on the left. Let $z_0 \in V$ and assume that f is holomorphic in $V \backslash \{z_0\}$ and that is has a Laurent expansion

$$f(z) = \sum_{n=-\infty}^{N} a_n (z-z_0)^n$$

Theorem A.4. *Then*

$$\int_\gamma f dz = 2\pi i a_{-1}$$

Sketch of proof: Using Cauchy's integral theorem the integral is the same as the integral over a small circle around z_0. One checks that

$$\int_{\partial B_\varepsilon(z_0)} (z-z_0)^n dz = i\int_0^{2\pi} e^{inx} e^{ix} dx = \begin{cases} 0 & \text{if } n \neq -1 \\ 2\pi i & \text{if } n = -1. \end{cases}$$