Notes on

PDE and Modelling

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Summer Term 2020

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 physics literature:

- R. Feynman, Leighton, Sands: The Feynman lectures in physics.

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 2020. A current version can be found at the eCampus page of the course.

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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. Here c is the speed of light.

Theory of electromagnetic waves is a beautiful theory combining previous complicated special theories of magnetism, electromagnetic 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 loose 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 $|x|^{-1}$. Here $\hbar$ is the reduced Planck's constant,

$$\hbar \sim 1,054571817 \times 10^{-34} kg\, m^2/s.$$

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

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

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 electrons, 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 realized that particles behave like waves. The most intriguing thought experiment is the double slit experiment. If we fix the frequency (color) 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 pattern 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. Selfadjoint operators

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

4. Symmetry groups

5. Scattering

6. Multiparticle systems

2 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.

2.1 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

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

Definition 2.1. *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 2.2. *Suppose that $T \in L(X,Y)$ is invertible, .i.e. it has a two sided inverse. 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 $\|AB\|_{X\to X} \le \|A\|_{X\to X}\|B\|_{X\to X}$ we have $\|A^j\|_{X\to X} \le \|A\|^j_{X\to X}$. 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 2.3. *$T \in L(X,Y)$ 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.

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Lemma 2.4. *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

$$(T - z1)(\sum_{j=0}^{\infty}(z-z_0)^j(T-z_01)^{-j-1} = 1$$

if $T - z_0 1$ is invertible and $|z - z_0|$ small we obtain

$$\rho(T) \ni z \to x^*(T - z1)^{-1}x$$

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

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

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

The set $\rho(T)$ is open by Lemma 2.2, 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 $T - z_j 1$ 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 nontrivial null space, and then $p(T) - \lambda$ has a nontrivial 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

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

and by the first part for $\varepsilon > 0$ there exists n so that $\|T^j\| \le (r+\varepsilon)^j$ for $j \ge n$, hence also

$$\sigma(T^j) \subset \overline{B_{(r+\varepsilon)^j}(0)}$$

for all $\varepsilon > 0$, and thus also for $\varepsilon = 0$, hence

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

Now suppose that

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

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

$$\limsup_{n\to\infty} \|T^n\|^{1/n} \leq a. \tag{2.1}$$

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

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

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

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

which implies (2.1).

Similarly we prove that $\sigma(T)$ is not empty. Suppose it is empty. Then, by Lemma 2.2 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. □

2.2 The spectrum of normal operators 1

In this section we only consider 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 2.5. *Let $T \in L(H_1, H_2)$. Its adjoint is defined by*

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

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

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

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

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

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

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

Examples for normal operators are unitary operators since for U unitary

$$U^* U = 1 = U U^*$$

and multiplication operators: Let X be set and μ a measure on X, $f \in L^\infty(\mu)$,

$$H := L^2(\mu) \ni g \to Tg := fg \in L^2(\mu)$$

Then

$$T^* g = \bar{f} g$$

and

$$T^* T g = |f|^2 g = T T^* g.$$

Lemma 2.6. *Suppose that T is normal. Then*

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

As a consequence

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

Proof. Let T be normal. then

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

and hence

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

thus

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

Next

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

and hence

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

Similarly $\|T^{2j}\| = \|T^j\|^2$, hence

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

and with $j + k = 2^n$

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

hence all inequalities have to be equalities and

$$\|T^j\|_{H\to H} = \|H\|_{H\to H}^j$$

for $j \in \mathbb{N}$. The last statement follows now from Lemma 2.4.

□