Seminar on Schrödinger operators

Winter term 2022/23

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Time and Place of the seminar: will be discussed at the organizational meeting

Number of sessions: **15**

Available Dates 17.10., 24.10., 31.10., 7.11., 14.11., 21.11., 28.11., 5.12., 12.12., 19.12., 9.1., 16.1., 23.1., Fr 27.1., 15:15 in M009, 6.2.

Content

In the seminar we mainly follow Teschl's book [17]. The book starts with Part 0/Chapter 0 which collects – as the number indicates – some preliminaries before the main subject starts. We suggest that every participants scrolls through this chapter, and reads whatever is unknown to him/her.

Supplementary Talk no. 1: Foundations: Hilbert spaces *17.10.*
Chapter 1 of [17] collects some standard and basic facts about Hilbert spaces. The topics in this Chapter are all of central importance. In case you find a topic in Chapter 0 of [17] which is supposedly not known to the other participants, please also include this into the talk.

Supplementary Talk no. 2: Foundations: Quantum Mechanics *24.10.*
Will be fixed by the speaker

Talk no. 1: Self-adjoint operators. *31.10.*
[17, Sec. 2.2 to 2.6] Self-adjoint operators, Quadratic forms and Friedrichs extension, resolvent and spectra, orthogonal sums of operators, self-adjoint extensions.

Talk no. 2: Spectral theorem. *7.11.*
[17, Sec. 3.1 to 3.3] Explain and prove the spectral theorem (Theorem 3.7). A bit a simpler version may be found in [9, Kapitel X] – you may have a look at it in order to compare it, but we expect Teschl's proof to fit better.
Depending on how much time remains discuss different types of spectra (absolutely continuous, singular, singular, continuous, pure point, point spectrum, discrete, essential). Essential and discrete are the most important ones, but may only discussed in Sec. 6.4. of the [17]; the precise list of spectra discussed should be discussed later with the organizers and the speaker of Talk no. 6

Talk no. 3: Applications of the spectral theorem, Part 1. *14.11.*
[17, Sections 4.1–4.2] Explain following Section 4.1 how to use integral methods, prove and discuss Stone's theorem, and discuss how to solve Problem 4.1. The main results in Section 4.2 are Corollary 4.6, Corollary 4.7 and Theorem 4.8.

Supplementary Talk no. 3: Applications of the spectral theorem, Part 2 *21.11.*
[17, Sections 4.3–4.6] Section 4.3 to 4.5 discuss methods to estimate eigenvalues and eigenspaces. Tensor products as in Section 4.6 are helpful for multiparticle systems.

Supplementary Talk no. 4: Quantum dynamics *28.11.*
Section 5.1 in [17] contains some statements that might be helpful later on: Theorem 5.1 and Stone's theorem (Theorem 5.2) and it Corollary 5.3. In particular, we get a nice criterion for essential self-adjointness. If we do not give this talks and need this later, we can also discuss it in the talk where it is applied to. The RAGE theorem and the Trotter formula are good to have, but we do not expect them to play a major role in later parts of the seminar.

Talk no. 4: Perturbation theory for self-adjoint operators, Part 1. *5.12.*
[17, Sections 6.1–6.3] Relatively bounded operators and the Kato-Rellich theorem, compact operators, Hilbert-Schmidt and trace class operators.

Talk no. 5: Perturbation theory for self-adjoint operators, Part 2. *12.12.*
[17, Sections 6.4–6.5] Relatively compact operators and Weyl's theorem. If not discussed in Talk no. 3, then discuss the discrete and essential spectrum. Explain how to describe the essential spectrum in terms of singular Weyl sequences. Discuss Theorem 6.19 (Weyl) and Theorem 6.20. If time admits, explain how Theorem 6.19 by Weyl is used in order to show that the essential spectrum of a self-adjoint operator defined by a quadratic form remains unchanged if another quadratic form of "controlled size" is added (see Section 6.5., in particular Lemma 6.9).

Talk no. 6: Gelfand space tripels. *Friday, Jan 13th, 15:15 in M009*,
Discuss and introduce Gelfand tripels $(\mathcal{M}, L^2(\mathbb{R}^n), \mathcal{M}^*)$, also known as rigged Hilbert spaces. You should have in mind as main examples for $\mathcal{M}$ the standard spaces of test spaces for distributions[1], e.g. $\mathcal{D} = C_c^\infty(\mathbb{R}^n)$, $\mathcal{E} = C^\infty(\mathbb{R}^n)$ and the space of Schwartz functions $\mathcal{S}(\mathbb{R}^n)$. Discuss the concept of generalized eigenfunctions within $\mathcal{M}^*$. Then present (and prove if you have time) the spectral theorem in rigged spaces.
The main reference [4, Chapter I, Section 4]. If time is short, then be a bit sketchy with Subsection 4.4. An additional reference would be Section 7.9 from the German book [8], maybe including some part of the previous sections in Chapter 7 if needed for the talk. A further reference is [12, Section 16.7], in fact this might be the mathematically most interesting and modern reference from this list. Please consult the article [3] in order to decide which parts are most relevant to physics. As references for the theory of distributions, we recommend [F. Constantinescu, Distributionen und ihre Anwendungen in der Physik, Teubner] which is focused on applications in physics, or to [L. Jantscher, Distributionen, de Gryuter] and [W. Walter, Theorie der Distributionen, BI Wissenschaftsverlag] for more comprehensive treatments.

[1] Here it might be appropriate to say more about distributions

Supplementary Talk no. 5: The free Schrödinger operator und eindimensionale Schrödinger-Operatoren *19.12.*

The subject of this talk is [17, Chapter 7 and 9]. Section 7.1 summarize standard facts about the Fourier transformation and is assumed to be known. Section 7.2 determines the spectrum and the core of the Laplacian $H_0 = -\Delta$ and its core, which is viewed as the free Schrödinger operator. The time evolution of H_0 is studied in Section 7.3. For time reasons we skip Section 7.4 that treats the resolvent and Green's function.
From Chapter 9 we introduce the Sturm–Liouville operator and the Wronskian as in Section 9.1. If time admits, we introduce the conditions "limit circle" and "limit point" in Section 9.2, and summarize its main properties (Theorem 9.6, Theorem 9.9). Then continue in Section 9.7 as long as time admits. Theorem 9.38 can obviously not be proven, but its result would be interesting to present.

Talk no. 7: Algebraic identities, conserved quantities, Noether's theorem, Harmonic Oscillator. *9.1.*
The talk should describe algebraic methods for treating the Schrödinger equation and for studying the spectrum of the Schrödinger operator. This is the subject of [17, Chapter 8] whose essential parts should be explained. However, it seems that Teschl's book does not consider the full symmetry group we are interested in. The symmetry group is O(4) for the Schrödinger operator with Coulomb potential and SU(3) for the harmonic oscillator. For these extended symmetries and their consequences (higher multiplicities!) we refer to Schiff's book, more precisely [16, Pages 236–...] for the Coulomb potential and [16, Pages 239–... and Pages 209–212] for the harmonic oscillator. E.g. for the Coulomb potential, the obvious O(3) symmetry of a Schrödinger operator with central potential extends to an O(4) action. From the mathematical point of view, we should note, that Schiff's book only explains and discusses how to extend the induced Lie algebra representation of $\mathfrak{so}(3) = \mathfrak{o}(3)$ to a Lie algebra representation of the Lie algebra $\mathfrak{so}(4) = \mathfrak{o}(4) = \mathfrak{spin}(4) \cong \mathfrak{so}(3) \oplus \mathfrak{so}(3)$. To make it mathematically complete, note the following: Any Lie-algebra representation $\mathfrak{so}(d) = \mathfrak{spin}(d) \to \mathfrak{gl}(V) = \mathrm{End}(V)$ comes from a unique representation $\mathrm{Spin}(4) \to \mathrm{GL}(V)$. Now, one easily sees that the black commuting diagram of Lie groups and Lie group homomorphisms extends in a unique way to the full diagram, a so-called push-out diagram.

$$
\begin{tikzcd}
\mathrm{Spin}(3) \arrow[rr] \arrow[dr] \arrow[dd] & & \mathrm{Spin}(4) \arrow[dl] \arrow[dd] \\
& \mathrm{GL}(V) & \\
\mathrm{O}(3) \arrow[ur] \arrow[rr] & & \mathrm{O}(4) \arrow[ul, dashed]
\end{tikzcd}
$$

As orientation-reversing elements in $\mathrm{O}(d)$ might be more difficult to quantize,

we rather restict to $\mathrm{SO}(d)$ instead of $\mathrm{O}(d)$.
Be aware, that following Schiff's book the physical notation for elements of a Lie algebra are i times the elements of the mathematician's Lie-algebra. For examples: a mathemtician would say "$\mathfrak{su}(d)$ is the Lie alebra of $\mathrm{SU}(d)$ and consists of all traceless skew-hermitian matrices", while many physicists would say "$\mathrm{SU}(d)$" is infinitesimally generated by the traceless hermitian matrices."
Similar content in the Coulomb case might also be found in Merzbacher's book [13]. The treatment of the Coulomb case in Münster's book [14, Kapitel 13.2] puts more emphasis on operator methods.
In the case of the harmonic oscillator, I (Bernd Ammann) did not find Schiff's book that clear. Apparently, he extends the natural $\mathfrak{so}(3) = \mathfrak{su}(2)$-Lie algebra representation to an $\mathfrak{su}(3)$-Lie algebra action. The corresponding embedding $\mathfrak{su}(2) \hookrightarrow \mathfrak{su}(3)$ is <u>not</u> the one as an upper left block, with zero in the third line and column. It is the embedding of Lie algebras $\mathfrak{so}(3) \hookrightarrow \mathfrak{su}(3)$ given by complexification. This yields an embedding $\mathrm{SO}(3) \to \mathrm{SU}(3)$.
Maybe the best reference for explaining the $\mathrm{SU}(3)$-action for the harmonic oscillator case is the very old original article by Jauch and Hill [11]. It is brief, but has good aspects, and it generalizes to an $\mathrm{SU}(d)$-action on phase space of the d-dimensional harmonic oscillator, that extends the $\mathrm{SO}(d)$ action on configuration space. Using methods from symplectic geometry, one even sees that one even has an symplectic $\mathrm{U}(d)$-action preserving the Hamiltonian.[2]

Talk no. 8: One-particle Schrödinger operators. *16.1.*
The goal of this talk is [17, Chapter 10]. Please check whether Chapter 7 and 9 before are needed to understand this talk, and in case it does, please explain these results. In particular, determine the spectrum of the Schrödinger operator for hydrogen type atoms.

Talk no. 9: Atomic Schrödinger operators. *23.1.*
In contrast to the previous talk, we know consider now system out of several nuclei and electrons, as explained in [17, Chapter 11]. At first self-adjointnes is discussed. Then an important theorem is the HVZ-theorem (named after Zhislin, van Winter and Hunziker), which determines the essential spectrum of the atomic Schrödinger operator. An additional reference is [2, Section 3.3]. if time admits, also briefly summarize [2, Section 3.4].

Talk no. 10: The problem of self-adjointness. *Fr 27.1., 15:15 in M009*

We consider self-adjointness of $-\Delta - \frac{c}{r^2}$ and $D - \frac{c}{r}$. As both operators are self-adjoint in the formal sense, the question is mainly about the domain of these two operators. For operators $-\Delta - \frac{c}{r^2}$ or more generally $-\Delta + V(r)$ we recomment [2, Chapter 1]. For the Dirac operator see also [18, Subsection 1.4.4] for the free case, and [18, Section 5.3] for the general case.

[2] It remains obscure why the additional central $\mathbb{R}$-factor is not considered further in the literature: maybe it is not useful for quantum mechanical applications, maybe it is not a "Hamiltonian action" and maybe this is important to get a corresponding operator in quantum mechanics?

Talk no. 11: Regularity of eigenvalues of Coulomb type Schrödinger operators. *6.2.*

The literature for this talk will be given later

Further sources close to the subject

[2], [15], [1], [19], [8], [18], [14], [10], [5], [9], [5], [6], [7],

Seminar-Homepage

`https://ammann.app.uni-regensburg.de/lehre/2022w_schroedinger`

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