Topics in PDE (Winter term 2020/21)

July 16, 2019

Lectures/Exercises: Wed/Thu 16.45-18.15, starting on October 21, 2020

Motivation

Physical systems on length scales of the order $10^{-10}m$ are described by *quantum mechanics*, i.e., their time evolution obeys *Schrödinger's equation* which reads

$$\begin{cases} -i\partial_t \psi(x,t) = (-\Delta + V)\psi(x,t)\,, \quad (x,t) \in \mathbb{R}^d \times \mathbb{R} \\ \psi(\cdot, 0) = \psi_0 \end{cases} \tag{1}$$

for one particle in the field of a potential V. Examples of such systems include *large atoms*, *molecules* or *(quasi)periodic systems* such as metals, semiconductors, and insulators. However, due to the large number of involved degrees of freedom (think of a single uranium atom for instance), solving the Schrödinger equation for such systems is out of reach (both analytically and numerically). In fact, already the Schrödinger equation for one nucleus at rest with two electrons orbiting around it (Helium in the Born–Oppenheimer approximation) cannot be solved analytically anymore and numerical schemes collapse already for 10 electrons or more. For this reason, one is in need of certain approximations. Typically, one wishes the approximation to be a "one-particle theory" with a certain "mean-field" which takes into account all the interactions between all the involved particles. Although the approximating theory will then usually be non-linear (in the sense that the mean-field depends on the solution of the Schrödinger equation, such as $-i\partial_t\psi = (-\Delta + \lambda|\psi|^3)\psi)$, the resulting Schrödinger equation can be handled, e.g., using *methods of functional analysis and PDE*.

In this course, we will already assume that we are given such a one-particle theory. In fact, we will assume that the potential does not even depend on the solution anymore! Our goal then is to understand properties of solutions of Schrödinger's equation (1). Unsurprisingly, the actual and the generalized *eigenfunctions of the Schrödinger operator* $H = -\Delta + V$ play a crucial role in this problem. These are the solutions of the *stationary Schrödinger equation*. The main techniques involved in this quest stem from functional analysis and partial differential equations. Our main goals here are two-fold.

1. First we give a brief (but hopefully sufficient general) overview of spectral theory of self-adjoint operators in Hilbert spaces. In particular, we discuss different spectral types $\sigma_{ac}, \sigma_{sc}, \sigma_{pp}$ of self-adjoint operators (Lebesgue decomposition and Borel–Stieltjes transform) and give dynamical (and thereby intimately physical) characterizations (RAGE).

2. The second goal is to show that the "unphysical" part σ_{sc} is empty under "physically reasonable conditions". (Although the reader should be warned that in fact the *existence of singular continuous spectrum is (Baire-type) generic*, see, e.g., Del Rio et al [4] and Simon [10]!) This will be established using techniques of *scattering theory*. The general goal of scattering theory is to show that states that are "asymptotically free" at times $t = -\infty$ will be asymptotically free again after they scatter away from the potential under suitable conditions on the potential. Physically, we want to show that for every vector f orthogonal to eigenvectors of H there exists a vector $f_0^{(\pm)}$ orthogonal to eigenvectors of H_0 such that $\lim_{t\to\pm\infty} \|u(t) - u_0(t)\| = 0$ where $u_0(0) = f_0^{(\pm)}$, $u(t) = \mathrm{e}^{-iHt} f$ and $u_0(t) = \mathrm{e}^{-it} f_0^{(\pm)}$ solves the free equation $-i\partial_t u_0 = H_0 u_0$. Mathematically this corresponds to perturbation theory on the (absolutely) continuous spectrum (which is in fact not very stable (unlike σ_{ess}), see the Theorem of Weyl and Neumann which is contained, e.g., in Kato [7, Chapter X, Theorems 2.1-2.3]) and manifests itself in the existence and completeness (whatever that means) of the *Møller wave operators* $\Omega_\pm(H, H_0) = s - \lim_{t\to\pm\infty} \mathrm{e}^{iHt}\mathrm{e}^{-iH_0 t} P_0^{ac}$ and the existence of an *eigenfunction expansion*. The latter means that any vector $f \in L^2(\mathbb{R}^d)$ can be represented as

$$f = \sum_{\lambda\in\sigma_{pp}} |\psi_\lambda\rangle\langle\psi_\lambda|f\rangle + \int_{\mathbb{R}^d} |\phi_\xi\rangle\langle\phi_\xi|f\rangle\, d\xi$$

where ψ_λ are the L^2-normalized eigenfunctions of H, i.e., $H\psi_\lambda = \lambda\psi_\lambda$, and ϕ_ξ solves the Lippman–Schwinger equation

$$\phi_{\xi_\lambda} = u_\pm - R_0(\lambda \mp i0) V \phi_{\xi_\lambda}$$

where

$$\hat{u}_\pm = v_\pm \delta(P_0 - \lambda) = v_\pm d\sigma_{S_\lambda} \quad v_\pm \in L^2(S_\lambda, |\nabla P_0(\xi)| d\sigma_\lambda)$$

with $S_\lambda = \{\xi \in \mathbb{R}^d :\, P_0(\xi) = \lambda\}$. (In our situation, $P_0(\xi) = \xi^2$.) Writing

$$\int_{\mathbb{R}^d} |\phi_\xi\rangle\langle\phi_\xi|f\rangle\, d\xi = \int_0^\infty d\lambda \int_{S_\lambda} d\sigma_{S_\lambda}(\xi)\ |\phi_\xi\rangle\langle\phi_\xi|f\rangle = \int_0^\infty d\lambda\ F_{S_\lambda}^* F_{S_\lambda} f$$

with

$$(F_{S_\lambda} f)(\xi) = \langle\phi_\xi, f\rangle\,, \quad \xi \in S_\lambda = \{\xi \in \mathbb{R}^d :\, P_0(\xi) = \lambda\}$$

$$(F_{S_\lambda}^* g)(x) = \int_{S_\lambda} d\sigma_{S_\lambda}(\xi)\ \phi_{\xi(\lambda)}(x) g(\xi)\,, \quad x \in \mathbb{R}^d$$

reveals that scattering theory is intimately connected to the problem of *Fourier restriction*, a fact that has been exploited in remarkable papers by Agmon–Hörmander [1] and later Ionescu–Schlag [6]. Anyway, such eigenfunction expansions are of ultimate interest in that they provide us with a basis of solutions of the stationary Schrödinger equation that can be used to understand solutions of the full Schrödinger equation (1).

(Preliminary) list of topics

1. Repetition on unbounded operators on Hilbert spaces (closed operators, adjoint operators, self-adjoint operators, resolvents and spectra, Kato–Rellich, quadratic forms (Friedrichs extension), KLMN) (Teschl [13, Sections 2.2-2.4, 6.1, 6.5] and Zenk [16, Sections 2.1-2.3, 3.5])

2. Borel measures and Lebesgue decomposition theorem (Amrein [3, Section 4.1], Reed–Simon [8, Section I.4], Teschl [13, Section 3.2])

3. Borel–Stieltjes transforms of measures (Simon [11, Section 11.1], Teschl [13, Section 3.4])

4. Spectral measures, spectral calculus, and spectral theorem (Amrein [3, Sections 4.2 and 4.4], Teschl [13, Section 3.1])

5. Spectral types, σ_{ac}, σ_{sc}, and σ_{pp} (Amrein [3, Section 4.3], Teschl [13, Section 3.3]

6. Dynamic characterization of the spectrum (Wiener, Strichartz–Last, RAGE) (Aizenman–Warzel [2, Sections 2.2-2.4])

7. σ_{disc} and σ_{ess} (Weidmann [14, Section 8.5])

8. Perturbation theory (Weyl's theorem, Kato's analytic perturbation theory of σ_{disc}, Weyl–Neumann example on instability of σ_{ac}, rank-one perturbations, Aronszajn–Donoghue theory, Simon–Wolff criterion) (Kato [7], Reed–Simon [9, Chapter XII], Simon–Wolff [12], Simon [11, Chapters 11-12] Teschl [13, Sections 6.4], Weidmann [14, Sections 9.1-9.2])

9. Convergence of resolvents (Reed–Simon [8, Section VIII.7], Teschl [13, Section 6.6], Weidmann [14, Section 9.3])

10. Scattering theory and absence of σ_{sc} for short range potentials (Agmon–Hörmander [1], Hörmander [5, Chapter XIV], Ionescu–Schlag [6], Reed–Simon [9, Sections XIII.6-7], Yafaev [15])

References

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