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Konrad Schmüdgen

# Unbounded Self-adjoint Operators on Hilbert Space

 Springer

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*To ELISA*

# Preface and Overview

This book is designed as an advanced text on unbounded self-adjoint operators in Hilbert space and their spectral theory, with an emphasis on applications in mathematical physics and various fields of mathematics. Though in several sections other classes of unbounded operators (normal operators, symmetric operators, accretive operators, sectorial operators) appear in a natural way and are developed, the leitmotif is the class of *unbounded self-adjoint operators*.

Before we turn to the aims and the contents of this book, we briefly explain the two main notions occurring therein. Suppose that  $\mathcal{H}$  is a Hilbert space with scalar product  $\langle \cdot, \cdot \rangle$  and  $T$  is a linear operator on  $\mathcal{H}$  defined on a dense linear subspace  $\mathcal{D}(T)$ . Then  $T$  is said to be *it symmetric* if

$$\langle Tx, y \rangle = \langle x, Ty \rangle \quad \text{for } x, y \in \mathcal{D}(T). \quad (0.1)$$

The operator  $T$  is called *self-adjoint* if it is symmetric and if the following property is satisfied: Suppose that  $y \in \mathcal{H}$  and there exists a vector  $u \in \mathcal{H}$  such that  $\langle Tx, y \rangle = \langle x, u \rangle$  for all  $x \in \mathcal{D}(T)$ . Then  $y$  lies in  $\mathcal{D}(T)$ . (Since  $\mathcal{D}(T)$  is assumed to be dense in  $\mathcal{H}$ , it follows then that  $u = Ty$ .)

Usually it is easy to verify that Eq. (0.1) holds, so that the corresponding operator is symmetric. For instance, if  $\Omega$  is an open bounded subset of  $\mathbb{R}^d$  and  $T$  is the Laplacian  $\Delta$  on  $\mathcal{D}(T) = C_0^\infty(\Omega)$  in the Hilbert space  $L^2(\Omega)$ , a simple integration-by-parts computation yields (0.1). If the symmetric operator is bounded, its continuous extension to  $\mathcal{H}$  is self-adjoint. However, for unbounded operators, it is often difficult to prove or not true (as in the case  $T = \Delta$ ) that a symmetric operator is self-adjoint. Differential operators and most operators occurring in mathematical physics are *not bounded*. Dealing with unbounded operators leads not only to many technical subtleties; it often requires the development of new methods or the invention of new concepts.

Self-adjoint operators are fundamental objects in mathematics and in quantum physics. The spectral theorem states that any self-adjoint operator  $T$  has an integral representation  $T = \int \lambda dE(\lambda)$  with respect to some unique spectral measure  $E$ . This gives the possibility to define functions  $f(T) = \int f(\lambda) dE(\lambda)$  of the operator and to develop a functional calculus as a powerful tool for applications. The spectrum

of a self-adjoint operator is always a subset of the reals. In quantum physics it is postulated that each observable is given by a self-adjoint operator  $T$ . The spectrum of  $T$  is then the set of possible measured values of the observable, and for any unit vector  $x \in \mathcal{H}$  and subset  $M \subseteq \mathbb{R}$ , the number  $\langle E(M)x, x \rangle$  is the probability that the measured value in the state  $x$  lies in the set  $M$ . If  $T$  is the Hamilton operator, the one-parameter unitary group  $t \rightarrow e^{itT}$  describes the quantum dynamics.

All this requires the operator  $T$  to be self-adjoint. For general symmetric operators  $T$ , the spectrum is no longer a subset of the reals, and it is impossible to get an integral representation  $T = \int \lambda dE(\lambda)$  or to define the exponentiation  $e^{iT}$ . That is, the distinction between symmetric operators and self-adjoint operators is crucial! However, many symmetric operators that are not self-adjoint can be extended to a self-adjoint operator acting on the same Hilbert space.

The main aims of this book are the following:

- to provide a detailed study of unbounded self-adjoint operators and their properties,
- to develop methods for proving the self-adjointness of symmetric operators,
- to study and describe self-adjoint extensions of symmetric operators.

A particular focus and careful consideration is on the technical subtleties and difficulties that arise when dealing with unbounded operators.

Let us give an overview of the contents of the book. Part I is concerned with the basics of unbounded closed operators on a Hilbert space. These include fundamental general concepts such as regular points, defect numbers, spectrum and resolvent, and classes of operators such as symmetric and self-adjoint operators, accretive and sectorial operators, and normal operators.

Our first main goal is the theory of spectral integrals and the spectral decomposition of self-adjoint and normal operators, which is treated in detail in Part II. We use the bounded transform to reduce the case of unbounded operators to bounded ones and derive the spectral theorem in great generality for finitely many strongly commuting unbounded normal operators. The functional calculus for self-adjoint operators developed here will be essential for the remainder of the book.

Part III deals with generators of one-parameter groups and semigroups, as well as with a number of important and technical topics including the polar decomposition, quasi-analytic and analytic vectors, and tensor products of unbounded operators.

The second main theme of the book, addressed in Part IV, is perturbations of self-adjointness and of spectra of self-adjoint operators. The Kato–Rellich theorem, the invariance of the essential spectrum under compact perturbations, the Aronszajn–Donoghue theory of rank one perturbations and Krein’s spectral shift and trace formula are treated therein. A guiding motivation for many results in the book, and in this part in particular, are applications to Schrödinger operators arising in quantum mechanics.

Part V contains a detailed and concise presentation of the theory of forms and their associated operators. This is the third main theme of the book. Here the central results are three representation theorems for closed forms, one for lower semi-bounded Hermitian forms and two others for bounded coercive forms and for sectorial forms. Other topics treated include the Friedrichs extension, the order relation

of self-adjoint operators, and the min–max principle. The results on forms are applied to the study of differential operators. The Dirichlet and Neumann Laplacians on bounded open subsets of  $\mathbb{R}^d$  and Weyl’s asymptotic formula for the eigenvalues of the Dirichlet Laplacian are developed in detail.

The fourth major main theme of the book, featured in Part VI, is the self-adjoint extension theory of symmetric operators. First, von Neumann’s theory of self-adjoint extensions, and Krein’s theory and the Ando–Nishio theorem on positive self-adjoint extensions are investigated. The second chapter in Part VI gives an extensive presentation of the theory of boundary triplets. The Krein–Naimark resolvent formula and the Krein–Birman–Vishik theory on positive self-adjoint extensions are treated in this context. The two last chapters of Part VI are concerned with two important topics where self-adjointness and self-adjoint extensions play a crucial role. These are Sturm–Liouville operators and the Hamburger moment problem on the real line.

Throughout the book applications to Schrödinger operators and differential operators are our guiding motivation, and while a number of special operator-theoretic results on these operators are presented, it is worth stating that this is not a research monograph on such operators. Again, the emphasis is on the *general theory of unbounded self-adjoint Hilbert space operators*. Consequently, basic definitions and facts on such topics as Sobolev spaces are collected in an appendix; whenever they are needed for applications to differential operators, they are taken for granted.

This book is an outgrowth of courses on various topics around the theory of unbounded self-adjoint operators and their applications, given for graduate and Ph.D. students over the past several decades at the University of Leipzig. Some of these covered advanced topics, where the material was mainly to be found in research papers and monographs, with any suitable advanced text notably missing. Most chapters of this book are drawn from these lectures. I have tried to keep different parts of the book as independent as possible, with only one exception: The functional calculus for self-adjoint operators developed in Sect. 5.3 is used as an essential tool throughout.

The book contains a number of important subjects (Krein’s spectral shift, boundary triplets, the theory of positive self-adjoint extensions, and others) and technical topics (the tensor product of unbounded operators, commutativity of self-adjoint operators, the bounded transform, Aronzajn–Donoghue theory) which are rarely if ever presented in text books. It is particularly hoped that the material presented will be found to be useful for graduate students and young researchers in mathematics and mathematical physics.

Advanced courses on unbounded self-adjoint operators can be built on this book. One should probably start with the general theory of closed operators by presenting the core material of Sects. 1.1, 1.2, 1.3, 2.1, 2.2, 2.3, 3.1, and 3.2. This could be followed by spectral integrals and the spectral theorem for unbounded self-adjoint operators based on selected material from Sects. 4.1, 4.2, 4.3 and 5.2, 5.3, avoiding technical subtleties. There are many possibilities to continue. One could choose relatively bounded perturbations and Schrödinger operators (Chap. 8), or positive form and their applications (Chap. 10), or unitary groups (Sect. 6.1), or von Neumann’s



extension theory (Sects. 13.1, 13.2), or linear relations (Sect. 14.1) and boundary triplets (Chap. 14). A large number of special topics treated in the book could be used as a part of an advanced course or a seminar.

The prerequisites for this book are the basics in functional analysis and of the theory of bounded Hilbert space operators as covered by a standard one semester course on functional analysis, together with a good working knowledge of measure theory. The applications on differential operators require some knowledge of ordinary and partial differential equations and of Sobolev spaces. In Chaps. 9 and 16 a few selected results from complex analysis are also needed. For the convenience of the reader, we have added six appendices; on bounded operators and classes of compact operators, on measure theory, on the Fourier transform, on Sobolev spaces, on absolutely continuous functions, and on Stieltjes transforms and Nevanlinna functions. These collect a number of special results that are used at various places in the text. For the results, here we have provided either precise references to standard works or complete proofs.

A few general notations that are repeatedly used are listed after the table of contents. A more detailed symbol index can be found at the end of the book. Occasionally, I have used either simplified or overlapping notations, and while this might at first sight seem careless, the meaning will be always clear from the context. Thus the symbol  $x$  denotes a Hilbert space vector in one section and a real variable or even the function  $f(x) = x$  in others.

A special feature of the book is the inclusion of numerous examples which are developed in detail and which are accompanied by exercises at the ends of the chapters. A number of simple standard examples (for instance, multiplication operators or differential operators  $-i\frac{d}{dx}$  or  $-\frac{d^2}{dx^2}$  on intervals with different boundary conditions) are guiding examples and appear repeatedly throughout. They are used to illustrate various methods of constructing self-adjoint operators, as well as new notions even within the advanced chapters. The reader might also consider some examples as exercises with solutions and try to prove the statements therein first by himself, comparing the results with the given proofs. Often statements of exercises provide additional information concerning the theory. The reader who is interested in acquiring an ability to work with unbounded operators is of course encouraged to work through as many of the examples and exercises as possible. I have marked the somewhat more difficult exercises with a star. All stated exercises (with the possible exception of a few starred problems) are really solvable by students, as can be attested to by my experience in teaching this material. The hints added to exercises always contain key tricks or steps for the solutions.

In the course of teaching this subject and writing this book, I have benefited from many excellent sources. I should mention the volumes by Reed and Simon [RS1, RS2, RS4], Kato's monograph [Ka], and the texts (in alphabetic order) [AG, BSU, BEH, BS, D1, D2, DS, EE, RN, Yf, We]. I have made no attempt to give precise credit for a result, an idea or a proof, though the few names of standard theorems are stated in the body of the text. The notes at the end of each part contain some (certainly incomplete) information about a few sources, important papers and monographs in this area and hints for additional reading. Also I have listed a number

of key pioneering papers. I felt it might be of interest for the reader to look at some of these papers and to observe, for instance, that H. Weyl's work around 1909–1911 contains fundamental and deep results about Hilbert space operators, while the corresponding general theory was only developed some 20 years later!

I am deeply indebted to Mr. René Gebhardt who read large parts of this book carefully and made many valuable suggestions. Finally, I would like to thank D. Dubray and K. Zimmermann for reading parts of the manuscript and Prof. M.A. Dritschel and Dr. Y. Savchuk for their help in preparing this book.

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Konrad Schmüdgen

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# General Notation

- $\mathbb{N}_0$ : set of nonnegative integers,  
 $\mathbb{N}$ : set of positive integers,  
 $\mathbb{Z}$ : set of integers,  
 $\mathbb{R}$ : set of real numbers,  
 $\mathbb{C}$ : set of complex numbers,  
 $\mathbb{T}$ : set of complex numbers of modulus one,  
 $i$ : complex unit,  
 $\chi_M$ : characteristic function of a set  $M$ .

For  $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d$ ,  $k = 1, \dots, d$ , and  $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ , we set

$$\begin{aligned}
 x^\alpha &:= x_1^{\alpha_1} \cdots x_d^{\alpha_d}, & |\alpha| &:= \alpha_1 + \cdots + \alpha_d, \\
 \partial_k &:= \frac{\partial}{\partial x_k}, & D_k &:= -i \frac{\partial}{\partial x_k}, \\
 \partial^\alpha &:= \partial_1^{\alpha_1} \cdots \partial_d^{\alpha_d} = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_d}}{\partial x_d^{\alpha_d}}, \\
 D^\alpha &:= D_1^{\alpha_1} \cdots D_d^{\alpha_d} = (-i)^{|\alpha|} \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_d}}{\partial x_d^{\alpha_d}}
 \end{aligned}$$

with the convention that terms with  $\alpha_j = 0$  are set equal to one.

Sequences are written by round brackets such as  $(x_n)_{n \in \mathbb{N}}$  or  $(x_n)$ , while sets are denoted by braces such as  $\{x_i : i \in I\}$ . Pairs of elements are written as  $(x, y)$ .

For an open subset  $\Omega$  of  $\mathbb{R}^d$ ,

- $C^n(\Omega)$  is the set of  $n$  times continuously differentiable complex functions on  $\Omega$ ,  
 $C_0^\infty(\Omega)$  is the set of functions in  $C^\infty(\Omega)$  whose support is a compact subset of  $\Omega$ ,  
 $C^n(\overline{\Omega})$  is the set of functions  $f \in C^n(\Omega)$  for which all functions  $D^\alpha f$ ,  $|\alpha| \leq n$ , admit continuous extensions to the closure  $\overline{\Omega}$  of the set  $\Omega$  in  $\mathbb{R}^d$ ,  
 $L^p(\Omega)$  is the  $L^p$ -space with respect to the Lebesgue measure on  $\Omega$ .

We write  $L^2(a, b)$  for  $L^2((a, b))$  and  $C^n(a, b)$  for  $C^n((a, b))$ .

“a.e.” means “almost everywhere with respect to the Lebesgue measure.”



The symbol  $\mathcal{H}$  refers to a Hilbert space with scalar product  $\langle \cdot, \cdot \rangle$  and norm  $\| \cdot \|$ . Scalar products are always denoted by angle brackets  $\langle \cdot, \cdot \rangle$ . Occasionally, indices or subscripts such as  $\langle \cdot, \cdot \rangle_j$  or  $\langle \cdot, \cdot \rangle_{H^2(\Omega)}$  are added.

The symbol  $\oplus$  stands for the orthogonal sum of Hilbert spaces, while  $\dot{+}$  means the direct sum of vector spaces. By a projection we mean an orthogonal projection.

- $\sigma(T)$ : spectrum of  $T$ ,
- $\rho(T)$ : resolvent set of  $T$ ,
- $\pi(T)$ : regularity domain of  $T$ ,
- $\mathcal{D}(T)$ : domain of  $T$ ,
- $\mathcal{N}(T)$ : null space of  $T$ ,
- $\mathcal{R}(T)$ : range of  $T$ ,
- $R_\lambda(T)$ : resolvent  $(T - \lambda I)^{-1}$  of  $T$  at  $\lambda$ ,
- $E_T$ : spectral measure of  $T$ .