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Philippe Blanchard
Erwin Brüning

Mathematical Methods in Physics

Distributions, Hilbert Space Operators, and Variational Methods

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Philippe Blanchard
University of Bielefeld
Faculty of Physics
Bielefeld, 33615
Germany

Erwin Brüning
University of Durban—Westville
Department of Mathematics
and Applied Mathematics
Durban, 4000
South Africa

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Dedicated to the memory of
Yurko Vladimir Glaser and Res Jost,
mentors and friends

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Preface

Courses in modern theoretical physics have to assume some basic knowledge of the theory of generalized functions (in particular distributions) and of the theory of linear operators in Hilbert spaces. Accordingly the Faculty of Physics of the University of Bielefeld offered a compulsory course *Mathematische Methoden der Physik* for students in the second semester of the second year which now has been given for many years. This course has been offered by the authors over a period of about ten years. The main goal of this course is to provide basic mathematical knowledge and skills as they are needed for modern courses in quantum mechanics, relativistic quantum field theory and related areas. The regular repetitions of the course allowed, on the one hand, testing of a number of variations of the material and on the other hand the form of the presentation. From this course the book *Distributionen und Hilbertraumoperatoren. Mathematische Methoden der Physik. Springer-Verlag Wien, 1993* emerged. The present book is a translated, considerably revised and extended version of this book. It contains much more than this course since we added many detailed proofs, many examples and exercises as well as hints linking the mathematical concepts or results to the relevant physical concepts or theories.

This book addresses students of physics who are interested in a conceptually and mathematically clear and precise understanding of physical problems, and it addresses students of mathematics who want to learn about physics as a source and as an area of application of mathematical theories, i.e., all those students with interest in the fascinating interaction between physics and mathematics.

It is assumed that the reader has a solid background in analysis and linear algebra (in Bielefeld this means three semesters of analysis and two of linear algebra). On this basis the book starts in Part A with an introduction to basic linear functional analysis as needed for the Schwartz theory of distributions and continues in Part B with the particularities of Hilbert spaces and the core aspects of the theory of linear operators in Hilbert spaces. Part C develops the basic mathematical foundations for modern computations of the ground state energies and charge densities in atoms and molecules, i.e., basic aspects of the direct methods of the calculus of variations including constrained minimization. A powerful strategy for solving linear and nonlinear boundary and eigenvalue problems, which covers the Dirichlet problem and its nonlinear generalizations, is presented as well. An appendix gives detailed proofs of the fundamental principles and results of functional analysis to the extent they are needed in our context.

With great pleasure we would like to thank all those colleagues and friends who have contributed to this book through their advice and comments, in particular G. Bolz, J. Loviscach, G. Roepstorff and J. Stubbe. Last but not least we thank the editorial team of Birkhäuser – Boston for their professional work.

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Ph. Blanchard
E. Brüning

Notation

$\mathbb{N}$	the natural numbers
$\mathbb{R}$	field of real numbers
$\mathbb{C}$	field of complex numbers
$\mathbb{K}$	field of real or of complex numbers
$\mathbb{R}_+$	the set of nonnegative real numbers
$\mathbb{K}^n$	$\mathbb{K}$ vector space of n-tuples of numbers in $\mathbb{K}$
$A \pm B$	$\{a \pm b;\ a \in A;\ b \in B\}$ for subsets A and B of a vector space V
ΛM	$\{\lambda \cdot u;\ \lambda \in \Lambda,\ u \in M\}$ for a subset $\Lambda \subset \mathbb{K}$ and a subset M of a vector space V over $\mathbb{K}$
$A \backslash B$	the set of all points in a set A which do not belong to the subset B of A
$\mathcal{C}(\Omega) = \mathcal{C}(\Omega; \mathbb{K})$	vector space of all continuous functions $f : \Omega \to \mathbb{K}$, for an open set $\Omega \subset \mathbb{K}^n$
supp f	support of the function f
$\mathcal{C}_0(\Omega)$	vector space of all continuous functions $f : \Omega \to \mathbb{K}$ with compact support in Ω
$\mathcal{C}^k(\Omega)$	vector space of all functions which have continuous derivatives up to order k, for $k = 0, 1, 2, \ldots$

$D^\alpha = \frac{\partial^{\lvert\alpha\rvert}}{\partial x_1^{\alpha_1}\cdots\partial x_n^{\alpha_n}}$	derivative monomial of order $\lvert\alpha\rvert = \alpha_1 + \cdots + \alpha_n$, defined on spaces $\mathcal{C}^k(\Omega)$, for open sets $\Omega \subset \mathbb{R}^n$ and $k \geq \lvert\alpha\rvert$
$\mathcal{D}_K(\Omega)$	vector space of all functions $f : \Omega \to \mathbb{K}$ which have continuous derivatives of any order and which have a compact support supp f contained in the compact subset $\mathbb{K}$ of $\Omega \subset \mathbb{R}^n$, equipped with the topology of uniform convergence of all derivatives
$\mathcal{D}(\Omega)$	inductive limit of the spaces $\mathcal{D}_K(\Omega)$ with respect to all subsets $K \subset \Omega$, K compact; test function space of all $\mathcal{C}^\infty$-functions $f : \Omega \to \mathbb{K}$ which have a compact support in the open set $\Omega \subset \mathbb{R}^n$
$\lvert x\rvert$	Euclidean norm $\sqrt{x_1^2 + \cdots + x_n^2}$ of the vector $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$
$\mathcal{S}(\Omega)$	test function space of all $\mathcal{C}^\infty$-functions $f : \Omega \to \mathbb{K}$ which, together with all their derivatives decrease faster than const. $(1 + \lvert x\rvert)^{-k}$ for $k = 0, 1, 2, \ldots$, for some constant and $x \in \Omega$
$\mathcal{E}(\Omega)$	test function space of all $\mathcal{C}^\infty$-functions $f : \Omega \to \mathbb{K}$, equipped with the topology of uniform convergence of all derivatives $f^\alpha = D^{(\alpha)} f$ on all compact subsets K of Ω
lctvs	locally convex topological vector space
hlctvs	Hausdorff locally convex topological vector space
X^*	algebraic dual of a vector space X
X'	topological dual of a topological vector space X
$\mathcal{D}'(\Omega) \equiv \mathcal{D}(\Omega)'$	space of all distributions on the open set $\Omega \subseteq \mathbb{R}^n$
$\mathcal{S}'(\Omega) \equiv \mathcal{S}(\Omega)'$	space of all tempered (i.e., slowly growing) distributions on $\Omega \subseteq \mathbb{R}^n$
$\mathcal{E}'(\Omega) \equiv \mathcal{E}(\Omega)'$	space of all distributions on $\Omega \subseteq \mathbb{R}^n$ with compact support
I_f	the regular distribution defined by the locally integrable function f
$\mathcal{D}'_{\mathrm{reg}}(\Omega)$	the space of all regular distributions on the open set $\Omega \subseteq \mathbb{R}^n$
$\mathcal{D}'_+(\mathbb{R})$	space of all distributions on $\mathbb{R}$ with support in $\mathbb{R}_+$
$L^p(\Omega)$	space of equivalence classes of Lebesgue measurable functions on $\Omega \subseteq \mathbb{R}^n$ for which $\lvert f\rvert^p$ is Lebesgue integrable over Ω; $1 \leq p < \infty$, Ω Lebesgue measurable

$L^\infty(\Omega)$ — space of all equivalence classes of Lebesgue measurable functions on Ω which are essentially bounded; $\Omega \subseteq \mathbb{R}^n$ Lebesgue measurable

$p_{K,m}$ — for $m = 0, 1, 2, \ldots$, $K \subset \Omega$, K compact, $\Omega \subseteq \mathbb{R}^n$ open, the semi-norm on $\mathcal{D}_K(\Omega)$ defined by

$$p_{K,m}(f) = \sup_{|\alpha| \le m,\, x \in K} |D^\alpha f(x)|$$

$q_{K,m}$ — the semi-norm on $\mathcal{D}_K(\Omega)$ defined by

$$q_{K,m}(f) = \left(\sum_{|\alpha| \le m} \int_K |D^\alpha f(x)|^2 dx \right)^{1/2}$$

K, m, Ω as above

$p_{m,k}$ — the norm on $\mathcal{S}(\mathbb{R}^n)$ defined by

$$p_{m,k}(f) = \sup_{x \in \mathbb{R}^n,\, |\alpha| \le k} (1 + x^2)^{\frac{m}{2}} |D^\alpha f(x)|$$

for $m, k = 0, 1, 2, \ldots$

$B_{p,r}(x_0)$ — open ball of radius $r > 0$ and centre x_0, with respect to the semi-norm p

δ_a — Dirac's delta distribution centered at $x = a \in \mathbb{R}^n$; for $a = 0$ we write δ instead of δ_0

θ — Heaviside function

$vp\frac{1}{x}$ — Cauchy's principal value

$\frac{1}{x \pm io}$ — $\lim_{\epsilon \searrow 0} \frac{1}{x \pm i\epsilon}$ in $\mathcal{D}'(\mathbb{R})$

$\operatorname{supp} T$ — support of a distribution T

$\operatorname{supp\,sing} T$ — singular support of a distribution T

$f \otimes g$ — tensor product of two functions f and g

$T \otimes S$ — tensor product of two distributions T and S

$\mathcal{D}(\mathbb{R}^n) \otimes \mathcal{D}(\mathbb{R}^m)$ — algebraic tensor product of the test function spaces $\mathcal{D}(\mathbb{R}^n)$ and $\mathcal{D}(\mathbb{R}^m)$

$\mathcal{D}(\mathbb{R}^n) \otimes_\pi \mathcal{D}(\mathbb{R}^m)$ — the space $\mathcal{D}(\mathbb{R}^n) \otimes \mathcal{D}(\mathbb{R}^m)$ equipped with the projective tensor product topology

$\mathcal{D}(\mathbb{R}^n) \tilde{\otimes}_\pi \mathcal{D}(\mathbb{R}^m)$ — completion of the space $\mathcal{D}(\mathbb{R}^n) \otimes_\pi \mathcal{D}(\mathbb{R}^m)$

$u * v$ — convolution of two functions u and v

$T * u$ — the convolution of a distribution $T \in \mathcal{D}'(\Omega)$ with a test function $u \in \mathcal{D}(\Omega)$; regularization of T

$T * S$	convolution of two distributions T and S, if defined
$\bar{\partial}$	the differential operator $\frac{1}{2}(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y})$ on $\mathcal{D}'(\mathbb{R}^2)$
$\mathcal{F}$	operator of Fourier transform, on $L^1(\mathbb{R}^n)$ or $\mathcal{S}(\mathbb{R}^n)$
$\mathcal{F}'$	Fourier transform on $\mathcal{S}'(\mathbb{R}^n)$
$< \cdot, \cdot >$	inner product on a vector space
$\Vert \cdot \Vert$	norm on a vector space
$l^2(\mathbb{K})$	Hilbert space of square summable sequences of numbers in $\mathbb{K}$
$M^{\perp}$	orthogonal complement of a set M in a Hilbert space
$\operatorname{lin} M$	the linear span of the set M in a vector space
$[M]$	the closure of $\operatorname{lin} M$ in a topological vector space, i.e., the smallest closed subspace which contains M
$\dim V$	dimension of a vector space V
$D(A)$	domain (of definition) of the (linear) operator A
$\ker A = N(A)$	the kernel or null-space of a linear operator A
$\operatorname{ran} A$	the range or set of values of a linear operator A
$\Gamma(A)$	graph of a linear operator A
A^*	the adjoint of the densely defined linear operator A
A_F	Friedrichs extension of the densely defined non-negative linear operator A
$A + B$	form sum of the linear operators A and B
$\mathcal{L}(X, Y)$	space of continuous linear operators $X \to Y$, X and Y topological vector space over the field $\mathbb{K}$
$\mathfrak{B}(\mathcal{H}) = \mathcal{L}(\mathcal{H}, \mathcal{H})$	space of bounded linear operators on a Hilbert space $\mathcal{H}$
$\hat{A} = (D, A)$	linear operator with domain D and rule of assignment A
$\mathcal{K}(\mathcal{H})$	space of compact operators on a Hilbert space $\mathcal{H}$
$\mathcal{P}(\mathcal{H})$	space of all orthogonal projections on a Hilbert space $\mathcal{H}$
$\mathcal{S}(\mathcal{H})$	space of all trace class operators on a Hilbert space $\mathcal{H}$
$\mathcal{U}(\mathcal{H})$	space of all unitary operators on a Hilbert space $\mathcal{H}$
$\rho(A)$	resolvent set of a linear operator A

$R_A(z)$	resolvent operator at the point $z \in \rho(A)$ for the linear operator A
$\sigma(A)$	$= \mathbb{C}\backslash\rho(A)$, spectrum of the linear operator A
$\sigma_p(A)$	point spectrum of A
$\sigma_c(A)$	$= \sigma(A)\backslash\sigma_p(A)$, continuous spectrum of A
$\sigma_d(A)$	discrete spectrum of A
$\sigma_{ac}(A)$	absolutely continuous spectrum of A
$\sigma_{sc}(A)$	singular continuous spectrum of A
$\mathcal{H}_p(A)$	discontinuous subspace of A
$\mathcal{H}_c(A)$	continuous subspace of A
$\mathcal{H}_{sc}(A)$	singular continuous subspace of a self-adjoint operator A
$\mathcal{H}_{ac}(A)$	$= \mathcal{H}_c(A) \cap \mathcal{H}_{sc}(A)^{\perp}$, absolute continuous subspace of a self-adjoint operator A
$\mathcal{H}_s(A)$	$= \mathcal{H}_p(A) \oplus \mathcal{H}_{sc}(A)$, singular subspace of a self-adjoint operator A
$\mathcal{M}_b(H)$	subspace of bounded states of a self-adjoint Schrödinger operator H
$\mathcal{M}_\infty(H)$	subspace of scattering states of H, H as above
proj_M	orthogonal projection operator onto the closed subspace M of a Hilbert space
$[f \leq r]$	for a function $f : M \to \mathbb{R}$ and $r \in \mathbb{R}$ the sub-level set $\{x \in M : f(x) \leq r\}$
$proj_K$	projection onto the closed convex subset K of a Hilbert space $\mathcal{H}$
$[f = c]$	for a function $f : M \to \mathbb{R}$ and $c \in \mathbb{R}$ the level set $\{x \in M : f(x) = c\}$
$f'(x) = D_x f = Df(x)$	the Fréchet derivative of a function $f : U \to F$ at a point $x \in U$, for $U \subset E$ open, E, F Banach spaces
$\mathcal{B}(E^{\times n}, F)$	the Banach space of all continuous n-linear operators $E^{\times n} = E \times \cdots \times E \to F$, for Banach spaces E, F
$\delta f(x_0, h)$	Gâteaux differential of a function $f : U \to F$ at a point $x_0 \in U$ in the direction $h \in E$, $U \subset E$ open, E, F Banach spaces
$\delta_{x_0} f(h)$	Gâteaux derivative of f at $x_0 \in U$, applied to $h \in E$

$\Delta^n f(x_0, h)$	$= \frac{d^n}{dt^n} f(x_0 + th)\|_{t=0}$, nth variation of a function f at the point x_0 in the direction h
$T_x M$	tangent space of the differential manifold M at the point $x \in M$

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