Pseudo-Differential Operators
Theory and Applications
7

Maurice A. de Gosson

Symplectic Methods in Harmonic Analysis and in Mathematical Physics

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Vol. 7

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Symplectic Methods in Harmonic Analysis and in Mathematical Physics

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2010 Mathematics Subject Classification: 35S, 81Q, 81S, 53D, 46B, 37J05, 70H05, 70H15

ISBN 978-3-7643-9991-7 e-ISBN 978-3-7643-9992-4
DOI 10.1007/978-3-7643-9992-4

Library of Congress Control Number: 2011934363

Cover design: deblik, Berlin

Printed on acid-free paper

Springer Basel AG is part of Springer Science+Business Media

www.birkhauser-science.com

Contents

Foreword xiii

Preface xv
Description of the book xv

Prologue xxi
Some notation xxi
The space $\mathcal{S}(\mathbb{R}^n)$ and its dual $\mathcal{S}'(\mathbb{R}^n)$ xxii
The Fourier transform xxiii

Part I Symplectic Mechanics

1 Hamiltonian Mechanics in a Nutshell
1.1 Hamilton's equations 3
1.1.1 Definition of Hamiltonian systems 3
1.1.2 A simple existence and uniqueness result 4
1.2 Hamiltonian fields and flows 6
1.2.1 The Hamilton vector field 6
1.2.2 The symplectic character of Hamiltonian flows 8
1.2.3 Poisson brackets 10
1.3 Additional topics 11
1.3.1 Hamilton–Jacobi theory 11
1.3.2 The invariant volume form 13
1.3.3 The problem of "Quantization" 16

2 The Symplectic Group
2.1 Symplectic matrices 20
2.1.1 Definition of the symplectic group 20
2.1.2 Symplectic block-matrices 20
2.1.3 The affine symplectic group 21
2.2 Symplectic forms 22
2.2.1 The notion of symplectic form 22

2.2.2 Differential formulation . . . 23
2.3 The unitary groups $U(n, \mathbb{C})$ and $U(2n, \mathbb{R})$ . . . 25
2.3.1 A useful monomorphism . . . 25
2.3.2 Symplectic rotations . . . 25
2.3.3 Diagonalization and polar decomposition . . . 26
2.4 Symplectic bases and Lagrangian planes . . . 28
2.4.1 Definition of a symplectic basis . . . 28
2.4.2 The Lagrangian Grassmannian . . . 29

3 Free Symplectic Matrices
3.1 Generating functions . . . 31
3.1.1 Definition of a free symplectic matrix . . . 31
3.1.2 The notion of generating function . . . 33
3.1.3 Application to the Hamilton–Jacobi equation . . . 35
3.2 A factorization result . . . 38
3.2.1 Statement and proof . . . 38
3.2.2 Application: generators of $\mathrm{Sp}(2n, \mathbb{R})$ . . . 39

4 The Group of Hamiltonian Symplectomorphisms
4.1 The group $\mathrm{Symp}(2n, \mathbb{R})$ . . . 41
4.1.1 Definition and examples . . . 41
4.2 Hamiltonian symplectomorphisms . . . 43
4.2.1 Symplectic covariance of Hamiltonian flows . . . 43
4.2.2 The group $\mathrm{Ham}(2n, \mathbb{R})$ . . . 44
4.3 The symplectic Lie algebra . . . 47
4.3.1 Matrix characterization of $\mathfrak{sp}(2n, \mathbb{R})$ . . . 48
4.3.2 The exponential mapping . . . 49

5 Symplectic Capacities
5.1 Gromov's theorem and symplectic capacities . . . 51
5.1.1 Statement of Gromov's theorem . . . 51
5.1.2 Proof of Gromov's theorem in the affine case . . . 52
5.2 The notion of symplectic capacity . . . 55
5.2.1 Definition and existence . . . 55
5.2.2 The symplectic capacity of an ellipsoid . . . 59
5.3 Other symplectic capacities . . . 61
5.3.1 The Hofer–Zehnder capacity . . . 61
5.3.2 The Ekeland–Hofer capacities . . . 62

6 Uncertainty Principles
6.1 The Robertson–Schrödinger inequalities 66
6.1.1 The covariance matrix 66
6.1.2 A strong version of the Robertson–Schrödinger uncertainty principle 67
6.1.3 Symplectic capacity and the strong uncertainty principle 70
6.2 Hardy's uncertainty principle 71
6.2.1 Two useful lemmas 72
6.2.2 Proof of the multi-dimensional Hardy uncertainty principle 74
6.2.3 Geometric interpretation 76

Part II Harmonic Analysis in Symplectic Spaces

7 The Metaplectic Group
7.1 The metaplectic representation 79
7.1.1 A preliminary remark, and a caveat 80
7.1.2 Quadratic Fourier transforms 80
7.2 The projection π^{Mp} 84
7.2.1 Precise statement 84
7.2.2 Dependence on $\hbar$ 85
7.3 Construction of π^{Mp} 87
7.3.1 The group $\mathrm{Diff}^{(1)}(n)$ 87
7.3.2 Construction of the projection 89

8 Heisenberg–Weyl and Grossmann–Royer Operators
8.1 Dynamical motivation, and definition 91
8.1.1 The displacement Hamiltonian 91
8.1.2 The Heisenberg–Weyl operators 93
8.1.3 The symplectic covariance property of the HW operators 95
8.2 The Heisenberg group 96
8.2.1 The canonical commutation relations 97
8.2.2 Heisenberg group and Schrödinger representation 98
8.2.3 The Stone–von Neumann theorem 100
8.3 The Grossmann–Royer operators 102
8.3.1 The symplectic Fourier transform 102
8.3.2 Definition of the Grossmann–Royer operators 104
8.3.3 Symplectic covariance 106

8.4 Weyl–Heisenberg frames 107
8.4.1 The notion of frame 108
8.4.2 Weyl–Heisenberg frames 111
8.4.3 A useful "dictionary" 113

9 Cross-ambiguity and Wigner Functions
9.1 The cross-ambiguity function 117
9.1.1 Definition of $A(\psi, \phi)$ 117
9.1.2 Elementary properties of the cross-ambiguity function 119
9.2 The cross-Wigner transform 120
9.2.1 Definition and first properties of $W(\psi, \phi)$ 120
9.2.2 Translations of Wigner transforms 122
9.3 Relations between $A(\psi, \phi)$, $W(\psi, \phi)$, and the STFT 123
9.3.1 Two simple formulas 123
9.3.2 The short-time Fourier transform 125
9.3.3 The Cohen class 126
9.4 The Moyal identity 128
9.4.1 Statement and proof 128
9.4.2 An inversion formula 130
9.5 Continuity and growth properties 132
9.5.1 Continuity of $A(\psi, \phi)$ and $W(\psi, \phi)$ 132
9.5.2 Decay properties of $A(\psi, \phi)$ and $W(\psi, \phi)$ 134

10 The Weyl Correspondence
10.1 The Weyl correspondence 137
10.1.1 First definitions and properties 137
10.1.2 Definition using the Wigner transform 140
10.1.3 Probabilistic interpretation 142
10.1.4 The kernel of a Weyl operator 144
10.2 Adjoints and products 146
10.2.1 The adjoint of a Weyl operator 146
10.2.2 Composition formulas 147
10.3 Symplectic covariance of Weyl operators 150
10.3.1 Statement and proof of the symplectic covariance property 150
10.3.2 Covariance under affine symplectomorphisms 151
10.4 Weyl operators as pseudo-differential operators 152
10.4.1 The notion of pseudo-differential operator 153
10.4.2 The kernel of a Weyl operator revisited 155
10.4.3 Justification in the case $a \in S^m$ 156

10.5 Regularity results for Weyl operators 158
10.5.1 Some general results 158
10.5.2 Symbols in L^q spaces 160

11 Coherent States and Anti-Wick Quantization
11.1 Coherent states 163
11.1.1 A physical motivation 163
11.1.2 Properties of coherent states 164
11.2 Wigner transforms of Gaussians 169
11.2.1 Some explicit formulas 169
11.2.2 The cross-Wigner transform of a pair of Gaussians 171
11.3 Squeezed coherent states 172
11.3.1 Definition and characterization 173
11.3.2 Explicit action of $\mathrm{Mp}(2n,\mathbb{R})$ on squeezed states 175
11.4 Anti-Wick quantization 177
11.4.1 Definition in terms of coherent states 178
11.4.2 The Weyl symbol of an anti-Wick operator 180
11.4.3 Some regularity results 181

12 Hilbert–Schmidt and Trace Class Operators
12.1 Hilbert–Schmidt operators 185
12.1.1 Definition and general properties 185
12.1.2 Hilbert–Schmidt operators on $L^2(\mathbb{R}^n)$ 188
12.2 Trace class operators 189
12.2.1 The trace of a positive operator 189
12.2.2 General trace class operators 193
12.3 The trace of a Weyl operator 198
12.3.1 Heuristic discussion 198
12.3.2 Some rigorous results 200

13 Density Operator and Quantum States
13.1 The density operator 205
13.1.1 Pure and mixed quantum states 206
13.2 The uncertainty principle revisited 210
13.2.1 The strong uncertainty principle for the density operator 210
13.2.2 Sub-Gaussian estimates 212
13.2.3 Positivity issues and the KLM conditions 215

Part III Pseudo-differential Operators and Function Spaces

14 Shubin's Global Operator Calculus
14.1 The Shubin classes 223
14.1.1 Generalities 223
14.1.2 Definitions and preliminary results 225
14.1.3 Asymptotic expansions of symbols 229
14.2 More general operators ... which are not more general! 230
14.2.1 More general classes of symbols 231
14.2.2 A reduction result 232
14.3 Relations between kernels and symbols 236
14.3.1 A general result 236
14.3.2 Application: Wigner and Rihaczek distributions 237
14.4 Adjoints and products 239
14.4.1 The transpose and adjoint operators 239
14.4.2 Composition formulas 240
14.5 Proof of Theorem 330 243

Part IV Applications

15 The Schrödinger Equation
15.1 The case of quadratic Hamiltonians 247
15.1.1 Preliminaries 248
15.1.2 Quadratic Hamiltonians 249
15.1.3 Exact solutions of the Schrödinger equation 252
15.2 The general case 254
15.2.1 Symplectic covariance as a characteristic property of Weyl quantization 254
15.2.2 Quantum evolution groups and Stone's theorem 256
15.2.3 Application to Schrödinger's equation 256

16 The Feichtinger Algebra
16.1 Definition and first properties 261
16.1.1 Definition of $S_0(\mathbb{R}^n)$ 262
16.1.2 First properties of $S_0(\mathbb{R}^n)$ 263
16.2 Invariance and Banach algebra properties 266
16.2.1 Metaplectic invariance of the Feichtinger algebra 266
16.2.2 The algebra property of $S_0(\mathbb{R}^n)$ 268
16.3 A minimality property for $S_0(\mathbb{R}^n)$ 270
16.3.1 Heisenberg–Weyl expansions 270
16.3.2 The minimality property 271

16.4 A Banach Gelfand triple . . . 271
16.4.1 The dual space $S_0'(\mathbb{R}^n)$ . . . 272
16.4.2 The Gelfand triple (S_0, L^2, S_0') . . . 273

17 The Modulation Spaces M_s^q
17.1 The L^q spaces, $1 \leq q < \infty$ . . . 275
17.1.1 Definitions . . . 275
17.1.2 Weighted L^q spaces . . . 278
17.2 The modulation spaces M_s^q . . . 281
17.2.1 Definition of M_s^q . . . 282
17.2.2 Metaplectic and Heisenberg–Weyl invariance properties . . . 284
17.3 The modulation spaces M_s^∞ . . . 285
17.3.1 The weighted spaces L_s^∞ . . . 285
17.3.2 The spaces M_s^∞ . . . 286
17.4 The modulation spaces $M_s^{\infty,1}$ . . . 287
17.4.1 Definition and first properties . . . 288
17.4.2 Weyl operators with symbols in $M_s^{\infty,1}$ . . . 290

18 Bopp Pseudo-differential Operators
18.1 Introduction and motivation . . . 292
18.1.1 Bopp pseudo-differential operators . . . 293
18.1.2 Bopp operators viewed as Weyl operators . . . 295
18.1.3 Adjoints and a composition formula . . . 297
18.1.4 Symplectic covariance of Bopp operators . . . 298
18.2 Intertwiners . . . 299
18.2.1 Windowed wavepacket transforms . . . 299
18.2.2 The intertwining property . . . 302
18.3 Regularity results for Bopp operators . . . 303
18.3.1 Boundedness results . . . 303
18.3.2 Global hypoellipticity properties . . . 304

19 Applications of Bopp Quantization
19.1 Spectral results for Bopp operators . . . 307
19.1.1 A fundamental property of the intertwiners . . . 307
19.1.2 Generalized eigenvalues and eigenvectors of a Bopp operator . . . 309
19.1.3 Application: the Landau problem . . . 312
19.2 Bopp calculus and deformation quantization . . . 314
19.2.1 Deformation quantization: motivation . . . 315
19.2.2 The Moyal product and bracket . . . 316

19.3 Non-commutative quantum mechanics 318
19.3.1 Background 318
19.3.2 The operators $\widetilde{T}_\omega(z_0)$ and F_ω 320

Bibliography 325

Index 335

Foreword

This book is partially based on a series of lectures I gave during the fall term 2009 at the NuHAG Institute at the University of Vienna. It therefore has a structure reminiscent of a "Lecture Notes" monograph. This means, among other things, that I have felt free to often repeat or recall some material, or definition, that has been given in a previous chapter – exactly as when one is confronted by a class, where it is appropriate to give a brief review of what has been said during last week's lecture. I hope that this will make the reading of this book easier and more enjoyable to a majority of students and colleagues.

To those of the readers, certainly numerous, who will find that this book is too long for what it is, and have already closed it, I say "good bye!". For the few who would have liked to read more about all or some topics I develop, and who deplore that I haven't expanded them more, I can only quote the great Austrian physicist Walter Thirring (I owe this citation to Karlheinz Gröchenig):

> ... There are three things that are easy to start but very difficult to finish. The first is a war. The second is a love affair. The third is a trill. To this may be added a fourth: a book.

Maurice A. de Gosson

This work is dedicated with all my love to Charlyne,
for her invaluable support and help.

Preface

Harmonic analysis is one of the most active and fastest growing parts of both pure and applied mathematics. It has gone far beyond its primary goal, which was to study the representation of functions or signals as superpositions of trigonometric functions (Fourier series). The interest in harmonic analysis has always been great because of the wealth of its applications, and it plays nowadays a central role in the study of signal theory and time-frequency analysis. Its interest in pure mathematics (especially in functional analysis) has been revived by the introduction of new functional spaces which are tools of choice for studying regularity properties of pseudo-differential operators and their applications to mathematical physics. Methods from symplectic geometry add power and scope to modern harmonic analysis; historically these methods were perhaps for the first time systematically used in Folland's seminal book [59].

The aim of the present book is to give a rigorous and modern treatment of various objects from harmonic analysis with a strong emphasis on the underlying symplectic structure (for instance symplectic and metaplectic covariance properties). More specifically we have in mind two audiences: the time-frequency community, and mathematical physicists interested in applications to quantum mechanics. The concepts and methods are presented in such a way that they should be easily accessible to students at the upper-undergraduate level (a certain familiarity with basic Fourier analysis and the elementary theory of distributions is assumed). Needless to say, this book can also be read with profit by more advanced readers, and can be used as a reference work by researchers in partial differential equations, harmonic analysis, and mathematical physics. (Several chapters are part of ongoing research and contain material that is usually not addressed in introductory texts. For instance Gromov's non-squeezing theorem from symplectic topology and its applications, or the theory of phase space pseudodifferential operators.)

Description of the book

This book is divided into parts and chapters, each devoted to a particular topic. They have been designed in such a way that the material of each chapter can be covered in a 90 minutes lecture (but this, of course, very much depends on the student's background). The parts can be read independently.

Part I: Symplectic Mechanics

- **Chapter 1** is intended to be a review of the main concepts from Hamiltonian mechanics; while it can be skipped by the reader wanting to advance rapidly in the mathematics of harmonic analysis on symplectic spaces, it is recommended as a reference for a better understanding of the reasons for which many concepts are introduced. For instance, the Hamiltonian approach leads to a very natural and "obvious" motivation for consideration of the Heisenberg–Weyl operators, and of the Weyl pseudo-differential calculus. Also, deformation quantization does not really make sense unless one understands the mechanical reasons which lie behind it. The main result of this first chapter is that Hamiltonian flows consist of symplectomorphisms (the physicist's canonical transformations). This is proven in detail using an elementary method, that of the "variational equation" (which is a misnomer, because there is per se nothing variational in that equation!). We also discuss other topics, such as Poisson brackets (which is helpful to understand the first steps of deformation quantization; Hamilton–Jacobi theory is also briefly discussed).
- In **Chapter 2** the basics of the theory of the symplectic group are developed in a self-contained way. Only an elementary knowledge of linear algebra is required for understanding of the topics of this chapter; the few parts where we invoke more sophisticated material such as differential forms can be skipped by the beginner. A particular emphasis is put on the machinery of free symplectic matrices and their generating functions, which are usually ignored in first courses. The consideration of this topic simplifies many calculations, and has the advantage of yielding the easiest approach to the theory of the metaplectic group. We also discuss classical topics, such as the identification of the unitary group with a subgroup of the symplectic group.
- In **Chapter 3** we refine our study of the symplectic group by introducing the notion of free symplectic matrix and its generating functions. Free symplectic matrices can be defined in several different ways. Their importance comes from the fact that they are in a sense the building blocks of the symplectic group: every symplectic matrix is the product (in infinitely many ways) of exactly two free symplectic matrices. This property in turn allows an easy construction of simple sets of generators for the symplectic group. Last – but certainly not least! – the notion of free symplectic matrix will be instrumental for our definition in Chapter 7 of the metaplectic representation.
- In **Chapter 4** we discuss the notion of symplectomorphism, which is a generalization to the non-linear case of the symplectic transformations introduced in the previous chapters. This leads us to define two very interesting groups $\mathrm{Symp}(2n,\mathbb{R})$ and $\mathrm{Ham}(2n,\mathbb{R})$, respectively the group of all symplectomorphisms, and that of all Hamiltonian symplectomorphisms. These groups, which are of great interest in current research in symplectic topology, are non-linear generalizations of the symplectic group $\mathrm{Sp}(2n,\mathbb{R})$. The group

$\mathrm{Ham}(2n, \mathbb{R})$ will play an important role in our derivation of Schrödinger's equation for arbitrary Hamiltonian functions.

- In **Chapter 5** we introduce new and very powerful tools from symplectic geometry and topology: Gromov's symplectic non-squeezing theorem, and the associated notion of symplectic capacity. The importance of these concepts (which go back to the mid 1980s, and for which Gromov got the Abel Prize in 2009) in applications has probably not yet been fully realized in mathematical analysis, and even less in mathematical physics.
- In **Chapter 6** we address a topic which belongs to both classical and quantum mechanics, namely uncertainties principles, and we do this from a topological point of view. We begin by discussing uncertainty principles associated with a quasi-probability distribution from a quite general point of view (hence applicable both to the classical and quantum cases), and introduce the associated notion of covariance matrix. This enables us to reformulate the strong version of the uncertainty principle in terms of symplectic capacities. This approach to both classical and quantum uncertainties is new and due to the author. It seems to be promising because it allows us to analyze uncertainties which are more general than those usually considered in the literature, and has led to the definition of "quantum blobs", which are symplectically invariant subsets of phase space with minimum symplectic capacity one-half of Planck's constant h. We also prove a multi-dimensional Hardy uncertainty principle, which says that a function and its Fourier transform cannot be simultaneously dominated by too sharply peaked Gaussians.

Part II: Harmonic Analysis in Symplectic Spaces

- **Chapter 7** is devoted to a detailed study of the metaplectic group $\mathrm{Mp}(2n, \mathbb{R})$ as a unitary representation in $L^2(\mathbb{R}^n)$ of the two-fold covering of the symplectic group $\mathrm{Sp}(2n, \mathbb{R})$. The properties of $\mathrm{Sp}(2n, \mathbb{R})$, as exposed in Chapters 2 and 3, allow us to identify the generators of the metaplectic group as "quadratic Fourier transforms", generalizing the usual Fourier transforms. We construct with great care the projection (covering) mapping from the metaplectic group to the symplectic group, having in mind our future applications to the Wigner transform and the Schrödinger equation. In the forthcoming chapters we will use systematically the properties of the metaplectic group, in particular when establishing symplectic/metaplectic covariance formulas in Weyl calculus and the theory of the Wigner transform.
- In **Chapter 8** we study two companions, the Heisenberg–Weyl and Grossmann–Royer operators. These operators can in a sense be viewed as "quantized" versions of, respectively, translation and reflection operators and are symplectic Fourier transforms of each other. We also discuss the related notion of Heisenberg group and algebra which play such an important role in harmonic analysis in phase space; our approach starts with the canonical commutation relations of quantum mechanics. We also define and briefly dis-

cuss the affine variant of the metaplectic group, namely the inhomogeneous metaplectic group $\mathrm{AMp}(2n, \mathbb{R})$ which is an extension by the Heisenberg–Weyl operators of the metaplectic group $\mathrm{Mp}(2n, \mathbb{R})$.

- In **Chapter 9** we study in great detail various algebraic and functional properties of the cross-ambiguity and cross-Wigner functions, which are concisely defined using the Heisenberg–Weyl and Grossmann–Royer operators introduced in the previous chapter. We discuss the relations with the short-time Fourier transform used in signal and time-frequency analysis. We also prove a useful inversion formula for the cross-Wigner transform; this formula plays an important role in the theory of Feichtinger's modulation spaces which will be studied later in this book.

Part III: Pseudo-differential Operators and Function Spaces

- In **Chapter 10** we present the basics of Weyl calculus, in particular the definition of the Weyl correspondence which plays such an important role both in the theory of pseudodifferential operators and in modern quantum mechanics of which it is one of the pillars. The chapter begins with an introductory section where the need for "quantization" is briefly discussed. We prove various formulas (in particular formulas for the adjoint of a Weyl operator, and that for the twisted symbol of the composition of two operators).
- In **Chapter 11** we take a close look at the notion of coherent states (they are elementary Gaussian functions); the properties of the metaplectic group allow us to give very explicit formulas for their natural extension, the squeezed coherent states, which play a pivotal role both in harmonic analysis and in quantum mechanics (especially in the subdiscipline known as quantum optics). This leads us naturally to the consideration of anti-Wick operators (also called Toeplitz or Berezin operators), of which we give the main properties.
- In **Chapter 12** we review two venerable topics from functional analysis: the theory of Hilbert–Schmidt and the associated theory of trace class operators. This will allow us to give a precise meaning to the notion of mixed quantum state in Chapter 13. We discuss in some detail the delicate procedure of calculating the trace. In particular we state and prove a result making legitimate the integration of the kernel when the operator is a Weyl pseudodifferential operator.
- In **Chapter 13** we give a rigorous definition of the notion of mixed quantum state, and of the associated density operators (called density matrices in quantum mechanics). The relation between density operators and the Wigner transform is made clear and fully exploited. We discuss the very delicate notion of positivity for the density operator. This is done by introducing the Kastler–Loupias–Miracle-Sole conditions, which we relate to the uncertainty principle. We also apply Hardy's uncertainty principle in its multi-dimensional form to the characterization of sub-Gaussian mixed states; the results are stated concisely using the notion of symplectic capacity.

- **Chapter 14** is of a rather technical nature. We introduce Shubin's global symbol classes, and the associated pseudo-differential operators. Shubin classes are of a greater use in quantum-mechanics than the ordinary Hörmander classes because their definition takes into account global properties of polynomial decrease in phase space. We discuss the notion of asymptotic expansion of the symbols, and show that operators which are at first sight much more general can be reduced to the case of ordinary pseudo-differential operators. We also study the notion of τ-symbol of a pseudo-differential, and give formulas allowing one to switch between different values of the parameter τ.

Part IV: Applications

- In **Chapter 15** we study a great classic of quantum mechanics, in fact one of its pillars: Schrödinger's time-dependent equation. We begin by showing that this equation can be derived from the theory of the metaplectic group when associated to a quadratic Hamiltonian function. In the second part of the chapter we generalize our construction to arbitrary Hamiltonian functions by using Stone's theorem on strongly continuous one-parameter groups of unitary operators together with the characteristic property of symplectic covariance of Weyl pseudo-differential calculus.
- **Chapters 16 and 17** are an introduction to Feichtinger's theory of modulation spaces. The elements ψ of these spaces are functions (or distributions) on $\mathbb{R}^n$ characterized by the property that the cross-Wigner transform $W(\psi, \phi)$ belongs to some weighted Banach space of integrable functions on $\mathbb{R}^{2n}$ for every "window" ϕ. The simplest example is provided by the Feichtinger algebra $M^1(\mathbb{R}^n)$ which is the smallest Banach algebra containing the Schwartz functions and being invariant under the action of the inhomogeneous group (Chapter 16). Since Feichtinger's algebra is a Banach algebra it can be used with profit as a substitute for the Schwartz space; it allows in particular, together with its dual, to define a Gelfand triple. Modulation spaces play a crucial role in time-frequency analysis and in the theory of pseudodifferential operators. Their importance in quantum mechanics has only been recently realized, and is being very actively investigated.
- **Chapter 18** is an introduction to a new topic, which we have called *Bopp calculus*. Bopp operators are pseudodifferential operators of a certain type acting on phase space functions or distributions. They are associated in a natural way to the usual Weyl operators by "Bopp quantization rules", $x \longrightarrow x + \frac{1}{2}i\hbar\partial_p$, $p \longrightarrow p - \frac{1}{2}i\hbar\partial_x$. These rules are often used heuristically by physicists working in the area of deformation quantization; this chapter gives a rigorous justification of these manipulations. We note that the theory of Bopp operators certainly has many applications in pure mathematics and physics (Schrödinger equation in phase space).
- In **Chapter 19** we give a few applications of Bopp calculus. We begin by studying spectral properties of Bopp operators, which we relate to those of

the corresponding standard Weyl operators. As an example we derive the energy levels and eigenfunctions of the magnetic operator (also called Landau operator). We thereafter show that Bopp pseudodifferential operators allow one to express deformation quantization in terms of a pseudodifferential theory; this has of course many technical and conceptual advantages since it allows us to easily prove deep results on "stargenvalues" and "stargenvectors". The book ends on a beginning: the application of Bopp operators to an emerging subfield of mathematics called "noncommutative quantum mechanics" (NCQM), which has its origins in the quest for quantum gravity.

Acknowledgement

This work has been financed by the Austrian Research Agency FWF (Projektnummer P20442-N13). I wish to express my thanks to Hans Feichtinger and Karlheinz Gröchenig for their help and support, and correcting my misunderstandings about modulation spaces. I am solely responsible for remaining errors. I also thank Franz Luef for many stimulating conversations about modulation spaces and related topics from time-frequency analysis; some parts of this book are based on joint work with him. Last – but not least! – many thanks to you, Charlyne, for having typed with competence and patience a great part of the manuscript and having given me the loving environment I needed to write this book.

Prologue

In this preliminary chapter we introduce some notation and recall basic facts from linear algebra and vector calculus.

Some notation

Let $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$.

- $M(m, \mathbb{K})$ is the algebra of all $m \times m$ matrices with entries in $\mathbb{K}$.
- $\mathrm{GL}(m, \mathbb{K})$ is the general linear group. It consists of all invertible matrices in $M(m, \mathbb{K})$.
- $\mathrm{SL}(m, \mathbb{K})$ is the special linear group: it is the subgroup of $\mathrm{GL}(m, \mathbb{K})$ consisting of all matrices with determinant equal to 1.
- $\mathrm{Sym}(m, \mathbb{K})$ is the vector space of all symmetric matrices in $M(m, \mathbb{K})$; it has dimension $\frac{1}{2}m(m+1)$; $\mathrm{Sym}_+(2n, \mathbb{R})$ is the subset of $\mathrm{Sym}(m, \mathbb{K})$ consisting of the positive definite symmetric matrices.

  The elements of $\mathbb{R}^m$ should be viewed as column vectors

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

when displayed; for typographic simplicity we will usually write $x = (x_1, \ldots, x_n)$ in the text. The Euclidean scalar product $\langle \cdot, \cdot \rangle$ and norm $|\cdot|$ on $\mathbb{R}^m$ are defined by

$$x \cdot y = x^T y = \sum_{j=1}^{m} x_j y_j .$$

The gradient operator in the variables $x_1, \ldots, x_n$ will be denoted by

$$\partial_x \quad \text{or} \quad \begin{pmatrix} \partial x_1 \\ \vdots \\ \partial x_m \end{pmatrix} .$$

Let f and g be differentiable functions $\mathbb{R}^m \longrightarrow \mathbb{R}^m$; in matrix form the chain rule is

$$\partial_x (g \circ f)(x) = (Df(x))^T \partial_x f(x) \tag{1}$$

where $Df(x)$ is the Jacobian matrix of f: if $f = (f_1, \ldots, f_m)$ is a differentiable mapping $\mathbb{R}^m \longrightarrow \mathbb{R}^m$ then

$$Df = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_m} \end{pmatrix}. \tag{2}$$

Let $y = f(x)$; we will indifferently use the notation $Df(x)$ for the Jacobian matrix at x. If f is invertible, the inverse function theorem says that

$$D(f^{-1})(y) = [Df(x)]^{-1}. \tag{3}$$

If $f : \mathbb{R}^m \longrightarrow \mathbb{R}$ is a twice continuously differentiable function, its Hessian calculated at a point x is the symmetric matrix of second derivatives

$$D^2 f(x) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}. \tag{4}$$

Notice that the Jacobian and Hessian matrices are related by the formula

$$D_x(\partial_x f)(x) = D_x^2 f(x). \tag{5}$$

Also note the following useful formulae:

$$\langle A\partial_x, \partial_x \rangle \, e^{-\frac{1}{2}\langle Mx,x\rangle} = [\langle MAMx, x\rangle - \operatorname{Tr}(AM)] \, e^{-\frac{1}{2}\langle Mx,x\rangle}, \tag{6}$$

$$\langle Bx, \partial_x \rangle \, e^{-\frac{1}{2}\langle Mx,x\rangle} = \langle MBx, x\rangle \, e^{-\frac{1}{2}\langle Mx,x\rangle}, \tag{7}$$

where A, B, and M are symmetric matrices.

The space $\mathcal{S}(\mathbb{R}^n)$ and its dual $\mathcal{S}'(\mathbb{R}^n)$

Very useful classes of functions and distributions are the so-called Schwartz space $\mathcal{S}(\mathbb{R}^n)$ and its dual $\mathcal{S}'(\mathbb{R}^n)$, which is the space of tempered distributions. In our context they are better adapted than the space $C_o^\infty(\mathbb{R}^n)$ of infinitely differentiable functions with compact support (the latter is not invariant under Fourier transform).

Definition 1. The space $\mathcal{S}(\mathbb{R}^n)$ consists of all infinitely differentiable functions $f : \mathbb{R}^n \longrightarrow \mathbb{C}$ such that for every pair (α, β) of multi-indices there exists a constant $C_{\alpha\beta} \geq 0$ such that

$$|x^\alpha \partial_x^\beta f(x)| \leq C_{\alpha\beta} \quad \text{for } x \in \mathbb{R}^n.$$

This condition is equivalent to the existence of $C'_{\alpha\beta} \geq 0$ such that

$$|\partial_x^\beta (x^\alpha f)(x)| \leq C'_{\alpha\beta} \quad \text{for } x \in \mathbb{R}^n.$$

The proof of the equivalence of the two conditions above is left to the reader; it readily follows – after some tedious calculations – from Leibniz's rule for the derivatives of a product.

Clearly $C_0^\infty(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n)$; the archetypical example of a function which belongs to $\mathcal{S}(\mathbb{R}^n)$ but not to $C_0^\infty(\mathbb{R}^n)$ is the Gaussian $f(x) = e^{-|x|^2}$; more generally the product of a Gaussian by a polynomial is in $\mathcal{S}(\mathbb{R}^n)$. Note that $\mathcal{S}(\mathbb{R}^n)$ actually is an algebra: the product of two elements of $\mathcal{S}(\mathbb{R}^n)$ is also in $\mathcal{S}(\mathbb{R}^n)$ (this readily follows from the chain rule). The formulae

$$\|f\|_{\alpha\beta}^{(1)} = \sup_{x \in \mathbb{R}^n} |x^\alpha \partial_x^\beta f(x)|,$$
$$\|f\|_{\alpha\beta}^{(2)} = \sup_{x \in \mathbb{R}^n} |\partial_x^\beta (x^\alpha f)(x)|$$

define equivalent families of semi-norms on $\mathcal{S}(\mathbb{R}^n)$; one shows that $\mathcal{S}(\mathbb{R}^n)$ becomes a Fréchet space for the topology thus defined.

The Fourier transform

Let $f : \mathbb{R}^n \longrightarrow \mathbb{C}$ be an absolutely integrable function

$$\|f\|_{L^1} = \int_{\mathbb{R}^n} |f(x)| dx < \infty;$$

we will write for short $f \in L^1(\mathbb{R}^n)$. By definition the Fourier transform $\mathcal{F}f = \widehat{f}$ is the function defined by

$$\widehat{f}(\xi) = \left(\tfrac{1}{2\pi}\right)^{n/2} \int_{\mathbb{R}^n} e^{-i\xi \cdot x} f(x) dx.$$

We will use in this book the following variant of the Fourier transform $\mathcal{F}$:

$$F\psi(x) = \left(\tfrac{1}{2\pi\hbar}\right)^{n/2} \int_{\mathbb{R}^n} e^{-ix \cdot x'} \psi(x') dx';$$

here $\hbar$ is a positive parameter, which one identifies in physics with Planck's constant divided by 2π: $\hbar = h/2\pi$ (the notation is due to the physicist Dirac). One proves (Riemann–Lebesgue lemma) that $\lim_{|\xi| \to \infty} \widehat{f}(\xi) = 0$.

One of the main properties of the Schwartz space (and of it dual) is that it is invariant by the Fourier transform:

$$\mathcal{F} : \mathcal{S}(\mathbb{R}^n) \longrightarrow \mathcal{S}(\mathbb{R}^n),$$
$$\mathcal{F} : \mathcal{S}'(\mathbb{R}^n) \longrightarrow \mathcal{S}'(\mathbb{R}^n).$$

This is in strong contrast with the case of $C_o^\infty(\mathbb{R}^n)$: the only compactly supported function (or distribution, for that matter) whose Fourier transform is also compactly supported is 0 (this is easily seen if one knows that the Fourier transform of a compactly supported function is analytic, and can thus never have compact support).

Proposition 2. *The Fourier transforms $\mathcal{F} : f \longmapsto \widehat{f}$ and $f \longmapsto Ff$ are invertible automorphisms of $\mathcal{S}(\mathbb{R}^n)$ which extends by duality into automorphisms of $\mathcal{S}'(\mathbb{R}^n)$ defined by*

$$\langle \widehat{f}, g\rangle = \langle f, \widehat{g}\rangle \ , \ \ \langle Ff, g\rangle = \langle f, Fg\rangle$$

for $f \in \mathcal{S}'(\mathbb{R}^n)$, $g \in \mathcal{S}(\mathbb{R}^n)$. The restriction of these automorphism to $L^2(\mathbb{R}^n)$ are unitary.

Proof. Let $f \in \mathcal{S}(\mathbb{R}^n)$; for $\alpha, \beta \in \mathbb{N}^n$ we have

$$\xi^\alpha \partial_\xi^\beta \widehat{f} = (-i)^{|\alpha|+|\beta|} \widehat{\partial_x^\alpha x^\beta f};$$

since $\partial_x^\alpha x^\beta f \in \mathcal{S}(\mathbb{R}^n)$ there exists a constant $C_{\alpha\beta} > 0$ such that $|\xi^\alpha \partial_\xi^\beta \widehat{f}(\xi)| \leq C_{\alpha\beta}$, hence $\widehat{f} \in \mathcal{S}(\mathbb{R}^n)$. That the Fourier transform is an invertible automorphism of $\mathcal{S}(\mathbb{R}^n)$ follows from the Fourier inversion formula. The two last statements easily follow from Plancherel's formula

$$\int_{\mathbb{R}^n} f(x)\widehat{g}(x)dx = \int_{\mathbb{R}^n} \widehat{f}(x)g(x)dx$$

and their proof is therefore left to the reader. □

Part I

Symplectic Mechanics

Chapter 1

Hamiltonian Mechanics in a Nutshell

This chapter is an introduction to the basics of Hamiltonian mechanics, with an emphasis on its symplectic formulation. It thus motivates the symplectic techniques which will be developed in the forthcoming chapters. In fact, Hamiltonian mechanics is historically the main motivation for the study of the symplectic group in particular, and of symplectic geometry in general. For complements and an extended study the reader can consult with profit the treatises by Abraham–Marsden [2] and Arnol'd [3]; an elementary introduction at the undergraduate level is the classical book by Goldstein [63] and its re-editions. (This book is written for physicists, however, and the mathematics is not always rigorous.)

Historically, Hamiltonian mechanics goes back to the early work of Hamilton and Lagrange; its symplectic formulation (as exposed in this chapter) is relatively recent; see Arnol'd [3] and Abraham et al. [1] for detailed accounts.

1.1 Hamilton's equations

We will use the notation $x = (x_1, \ldots, x_n)$, $p = (p_1, \ldots, p_n)$ for elements of $\mathbb{R}^n$ and $z = (x, p)$ for elements of $\mathbb{R}^{2n}$ (the "phase space"). When using matrix notation, x, p, z will always be viewed as column vectors.

1.1.1 Definition of Hamiltonian systems

Let H ("the Hamiltonian") be a real-valued function in $C^\infty(\mathbb{R}^{2n})$; more generally we will consider "time-dependent Hamiltonians" $H \in C^\infty(\mathbb{R}^{2n} \times \mathbb{R})$, functions of z and t.

Definition 3. The system of $2n$ ordinary differential equations

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial p_j}(x, p, t), \quad \frac{dp_j}{dt} = -\frac{\partial H}{\partial x_j}(x, p, t) \tag{1.1}$$

is called the *Hamilton equations* associated with H.

M.A. de Gosson, *Symplectic Methods in Harmonic Analysis and in Mathematical Physics*, Pseudo-Differential Operators 7, DOI 10.1007/978-3-7643-9992-4_1, © Springer Basel AG 2011

To simplify the discussion we will assume that for every $z_0 = (x_0, p_0)$ belonging to an open subset Ω of $\mathbb{R}^{2n}$, this system has a unique solution $t \longmapsto z(t) = (x(t), p(t))$ such that $z(0) = z_0$, defined for $-T \leq t \leq T$ where $T > 0$. (See Abraham–Marsden [2], Ch. 1, §2.1, for a general discussion of global existence and uniqueness, including the important notion of “flow box”.)

A basic example is the following; we state it in the case $n = 1$:

$$H(x,p) = \frac{p^2}{2m} + U(x) \tag{1.2}$$

where m is a positive constant (“the mass”) and U a smooth function (“the potential”). In this case Hamilton's equations are

$$\frac{dx}{dt} = \frac{p}{m} \quad , \quad \frac{dp}{dt} = -U'(x). \tag{1.3}$$

In physics one writes $v = p/m$ (it is the velocity) and dp/dt, so that these equations are just a restatement of Newton's second law, familiar from elementary physics; the quantity $p^2/2m$ is the “kinetic energy”. (We have discussed in some detail the physical interpretation of Hamilton's equations in [65].)

This example motivates the following definition:

Definition 4. Let $t \longmapsto z(t)$ be a solution of Hamilton's equations. The number $E(t) = H(z(t))$ is called the energy along the solution curve through $z_0 = z(0)$ at time t. When H is time-independent, we have $H(z(t)) = H(z(0))$ for every t. More generally, any function which is constant along the curves $t \longmapsto z(t)$ is called a “constant of the motion”.

That the energy E is a constant for time-independent Hamiltonians follows from the chain rule applied to $H(z(t))$, taking Hamilton's equations into consideration: setting $z = z(t)$ we have

$$\frac{d}{dt}H(z(t)) = \sum_{j=1}^{n} \frac{\partial H}{\partial x_j}(z)\frac{dx_j}{dt} + \frac{\partial H}{\partial p_j}(z)\frac{dp_j}{dt} = 0.$$

In the case of time-dependent Hamiltonians the same argument shows that

$$\frac{d}{dt}H(z(t),t) = \frac{\partial H}{\partial t}(z(t),t)$$

hence the energy $E(t) = H(z(t),t)$ is not a constant of the motion.

1.1.2 A simple existence and uniqueness result

Here is an existence result which is sufficient for many applications to physics. We assume that the Hamiltonian is time-independent and of the type

$$H(x,p) = \sum\nolimits_{j=1}^{n} \frac{p_j^2}{2m_j} + U(x)$$

where $U \in C^\infty(\mathbb{R}^n)$.

Proposition 5. *If $U \geq a$ for some constant a, then every solution of Hamilton's equations*

$$\frac{dx_j}{dt} = \frac{p_j}{m_j} \quad , \quad \frac{dp_j}{dt} = -\frac{\partial U}{\partial x_j}(x)$$

$(1 \leq j \leq n)$ *exists for all times (and is unique).*

Proof. In view of the local existence theory for ordinary differential equations it suffices to show that the solutions $t \longmapsto z(t)$ remain in bounded sets for finite times. Since Hamilton's equations are insensitive to the addition of a constant to the Hamiltonian we may assume $a = 0$, and rescaling if necessary the momentum and position coordinates it is no restriction neither to assume $m_j = 1$ for $1 \leq j \leq n$. For notational simplicity we moreover assume $n = 1$. Let thus $t \to z(t) = (x(t), p(t))$ be a solution curve of the equations

$$\frac{dx}{dt} = p \quad , \quad \frac{dp}{dt} = -\frac{\partial U}{\partial x}(x)$$

and let $E = H(z(t))$ be the energy; since $H \geq U$ we have $E \geq U(x(t))$. In view of the triangle inequality

$$|x(t)| \leq |x(0)| + |x(t) - x(0)| \leq |x(0)| + \int_0^t \left|\tfrac{d}{dt}x(s)\right| ds;$$

since $\frac{d}{dt}x(s) = p(s)$ and

$$p(t) = \sqrt{2(E - U(x(t))} \leq \sqrt{2E} \tag{1.4}$$

we have:

$$|x(t)| \leq |x(0)| + \int_0^t |p(s)|\, ds \leq |x(0)| + \int_0^t \sqrt{2(E - U(x(s))} ds$$

so that

$$|x(t)| \leq |x(0)| + t\sqrt{2E}. \tag{1.5}$$

The inequalities (1.4) and (1.5) show that for t in any finite time-interval $[0, T]$ the functions $t \longmapsto x(t)$ and $t \longmapsto p(t) = x(t)$, and hence $t \longmapsto z(t)$, stay forever in a bounded set. □

One can show (see [1], §4.1) that the conclusions of Proposition 5 still hold if one replaces the boundedness condition $U \geq a$ by the much weaker requirement

$$U(x) \geq a - b|x|^2 \quad \text{for} \quad b > 0$$

where a and b are some constants ($b > 0$). This condition cannot be very much relaxed; for instance one shows (ibid.) that already in the case $n = 1$ the solutions of the Hamilton equations for

$$H(x, p) = \frac{p^2}{2m} - \frac{\varepsilon^2}{8}x^{2+(4/\varepsilon)}$$

are not defined for all t if $\varepsilon > 0$.

1.2 Hamiltonian fields and flows

From now on we will use the following more compact notation, borrowed from mechanics: time derivatives (i.e., derivatives with respect to t) will be denoted by putting a dot over the letter standing for the function. For instance, $\dot{x}$ means dx/dt. Derivatives will in general be written as ∂_x, ∂_{x_j}, etc. instead of $\partial/\partial x$, $\partial/\partial x_j$. We will also freely use the notation ∂_x for the gradient $(\partial_{x_1}, \ldots, \partial_{x_n})$. Similarly, $\partial_z = (\partial_x, \partial_p)$ is the gradient in the $2n$ variables $z_1 = x_1, \ldots, z_n = x_n; z_{n+1} = p_1, \ldots, z_{2n} = p_n$.

The Hamilton equations (1.1) can be rewritten in compact form as

$$\dot{z} = J\partial_z H(z) \tag{1.6}$$

where J is the "standard symplectic matrix" defined by

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

where 0 and I are the $n \times n$ zero and identity matrices. That matrix will play an essential role in all of this book.

1.2.1 The Hamilton vector field

Assume first that H is a time-independent Hamiltonian function.

Definition 6. We call the vector field

$$X_H = J\partial_z H = (\partial_x H, -\partial_p H)$$

the "Hamilton vector field of H"; the operator $J\partial_z$ is called a "*symplectic gradient*".

It follows from the elementary theory of ordinary autonomous differential equations that the system (1.1) defines a flow (ϕ_t^H): by definition the function $t \longmapsto z(t) = \phi_t^H(z_0)$ is the solution of Hamilton's equations with $z(0) = z_0$ and we have

$$\phi_t^H \phi_{t'}^H = \phi_{t+t'}^H \ , \ \phi_0^H = I \tag{1.7}$$

when t, t' and $t + t'$ are in the interval $[-T, T]$. In particular each ϕ_t^H is a diffeomorphism such that $(\phi_t^H)^{-1} = \phi_{-t}^H$.

Definition 7. One says that (ϕ_t^H) is the flow generated by the Hamilton equations for H.

The Hamilton vector field is gradient-free:

$$\operatorname{div} X_H = \partial_x (\partial_p H) - \partial_p (\partial_x H) = 0$$