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Stephen J. Gustafson,
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Mathematical Concepts of Quantum Mechanics

量子力学中的数学概念

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Preface

The first fifteen chapters of these lectures (omitting four to six chapters each year) cover a one term course taken by a mixed group of senior undergraduate and junior graduate students specializing either in mathematics or physics. Typically, the mathematics students have some background in advanced analysis, while the physics students have had introductory quantum mechanics. To satisfy such a disparate audience, we decided to select material which is interesting from the viewpoint of modern theoretical physics, and which illustrates an interplay of ideas from various fields of mathematics such as operator theory, probability, differential equations, and differential geometry. Given our time constraint, we have often pursued mathematical content at the expense of rigor. However, wherever we have sacrificed the latter, we have tried to explain whether the result is an established fact, or, mathematically speaking, a conjecture, and in the former case, how a given argument can be made rigorous. The present book retains these features.

Prerequisites for this book are introductory real analysis (notions of vector space, scalar product, norm, convergence, Fourier transform) and complex analysis, the theory of Lebesgue integration, and elementary differential equations. These topics are typically covered by the third year in mathematics departments. The first and third topics are also familiar to physics undergraduates. Those unfamiliar with Lebesgue integration can think about Lebesgue integrals as if they were Riemann integrals. This said, the pace of the book is not a leisurely one and requires, at least for beginners, some amount of work.

Even in dealing with mathematics students we have found it useful, if not necessary, to review basic mathematical notions such as the spectrum of an operator, and the Gâteaux or variational derivative, which we needed for the course. Moreover, to make the book relatively self-contained, we recall and sometimes discuss the basic notions mentioned above. As a result, the text is interspersed with mathematical supplements which occupy in total about a third of the material. A mathematically sophisticated reader can skim through them, or skip them altogether, and concentrate on physical applications. On the other hand, readers familiar with the physical content of quantum mechanics, and who would like to enhance their mathematics, could concentrate on those detours and consider the physics chapters as an application of the mathematics in a familiar setting.

Though we tried to increase the complexity of the material gradually, we were not always successful, and first in Chapter 8, and then in Chapter 14, there is a leap in the level of sophistication required from the reader.

This book consists of fifteen main chapters and one supplementary chapter, Chapter 17. The latter chapter is more technical than the preceding material. We did not include many standard topics which are well-covered elsewhere. These topics are referenced in Chapter 18, where we also give some comments on the literature and further reading.

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Vancouver/Toronto,
September 2002

Stephen Gustafson
Israel Michael Sigal

Preface to the Second Printing

For the second printing, we corrected a few misprints and inaccuracies; for some help with this, we are indebted to B. Nachtergaele. We have also added a small amount of new material. In particular, Chapter 10, on perturbation theory via the Feshbach method, is new, as are the short sub-sections 8.9 and 9.12 concerning the Hartree approximation and Bose-Einstein condensation. We also note a change in terminology, from "point" and "continuous" spectrum, to the mathematically more standard "discrete" and "essential" spectrum, starting in Chapter 5.

Vancouver/Toronto,
July 2005

Stephen Gustafson
Israel Michael Sigal

Contents

1 Physical Background 1
- 1.1 The Double-Slit Experiment 1
- 1.2 Wave Functions 3
- 1.3 State Space 4
- 1.4 The Schrödinger Equation 4
- 1.5 Mathematical Supplement: Operators on Hilbert Spaces 6

2 Dynamics 11
- 2.1 Conservation of Probability 11
- 2.2 Existence of Dynamics 12
- 2.3 The Free Propagator 16
- 2.4 Mathematical Supplement: Operator Adjoints 17
- 2.5 Mathematical Supplement: the Fourier Transform 20
  - 2.5.1 Definition of the Fourier Transform 20
  - 2.5.2 Properties of the Fourier Transform 21
  - 2.5.3 Functions of the Derivative 22

3 Observables 25
- 3.1 Mean Values and the Momentum Operator 25
- 3.2 Observables 26
- 3.3 The Heisenberg Representation 27
- 3.4 Quantization 28
- 3.5 Pseudodifferential Operators 29

4 The Uncertainty Principle 31
- 4.1 The Heisenberg Uncertainty Principle 31
- 4.2 A Refined Uncertainty Principle 32
- 4.3 Application: Stability of Hydrogen 33

5 **Spectral Theory** ... 35
5.1 The Spectrum of an Operator ... 35
5.2 Functions of Operators and the Spectral Mapping Theorem ... 40
5.3 Applications to Schrödinger Operators ... 42
5.4 Spectrum and Evolution ... 47
5.5 Variational Characterization of Eigenvalues ... 49
5.6 Number of Bound States ... 54
5.7 Mathematical Supplement: Integral Operators ... 60

6 **Scattering States** ... 61
6.1 Short-range Interactions: $\mu > 1$ ... 62
6.2 Long-range Interactions: $\mu \leq 1$ ... 65
6.3 Wave Operators ... 65

7 **Special Cases** ... 69
7.1 The Infinite Well ... 69
7.2 The Torus ... 70
7.3 A Potential Step ... 70
7.4 The Square Well ... 72
7.5 The Harmonic Oscillator ... 73
7.6 A Particle on a Sphere ... 76
7.7 The Hydrogen Atom ... 76
7.8 A Particle in an External EM Field ... 79

8 **Many-particle Systems** ... 81
8.1 Quantization of a Many-particle System ... 81
8.2 Separation of the Centre-of-mass Motion ... 85
8.3 Break-ups ... 87
8.4 The HVZ Theorem ... 88
8.5 Intra- vs. Inter-cluster Motion ... 90
8.6 Existence of Bound States for Atoms and Molecules ... 92
8.7 Scattering States ... 93
8.8 Mathematical Supplement: Tensor Products ... 95
8.9 Appendix: Hartree and Gross-Pitaevski Equations ... 97

9 **Density Matrices** ... 103
9.1 Introduction ... 103
9.2 States and Dynamics ... 103
9.3 Open Systems ... 105
9.4 The Thermodynamic Limit ... 106
9.5 Equilibrium States ... 107
9.6 The $T \to 0$ Limit ... 107
9.7 Example: a System of Harmonic Oscillators ... 109
9.8 A Particle Coupled to a Reservoir ... 110
9.9 Quantum Systems ... 111

9.10 Problems 111
9.11 Hilbert Space Approach 111
9.12 BEC at T=0 113
9.13 Appendix: the Ideal Bose Gas 114
9.14 Appendix: Bose-Einstein Condensation 119
9.15 Mathematical Supplement: the Trace, and Trace Class Operators 122
9.16 Mathematical Supplement: Projections 127

10 Perturbation Theory: Feshbach Method 131
10.1 The Feshbach Method 132
10.2 Example: The Zeeman Effect 135
10.3 Example: Time-dependent Perturbations 137
10.4 Appendix: Proof of Theorem 10.1 142

11 The Feynman Path Integral 145
11.1 The Feynman Path Integral 145
11.2 Generalizations of the Path Integral 148
11.3 Mathematical Supplement: The Trotter Product Formula 149

12 Quasi-classical Analysis 151
12.1 Quasi-classical Asymptotics of the Propagator 152
12.2 Quasi-classical Asymptotics of Green's Function 156
12.2.1 Appendix 159
12.3 Bohr-Sommerfeld Semi-classical Quantization 159
12.4 Quasi-classical Asymptotics for the Ground State Energy 161
12.5 Mathematical Supplement: Operator Determinants 163

13 Mathematical Supplement: The Calculus of Variations 167
13.1 Functionals 167
13.2 The First Variation and Critical Points 169
13.3 Constrained Variational Problems 173
13.4 The Second Variation 174
13.5 Conjugate Points and Jacobi Fields 176
13.6 The Action of the Critical Path 179
13.7 Appendix: Connection to Geodesics 182

14 Resonances 185
14.1 Tunneling and Resonances 185
14.2 The Free Resonance Energy 187
14.3 Instantons 189
14.4 Positive Temperatures 191
14.5 Pre-exponential Factor for the Bounce 193
14.6 Contribution of the Zero-mode 195
14.7 Bohr-Sommerfeld Quantization for Resonances 195

15 Introduction to Quantum Field Theory 199
15.1 The Place of QFT 199
15.1.1 Physical Theories 200
15.1.2 The Principle of Minimal Action 200
15.2 Klein-Gordon Theory as a Hamiltonian System 201
15.2.1 The Legendre Transform 201
15.2.2 Hamiltonians 202
15.2.3 Poisson Brackets 202
15.2.4 Hamilton's Equations 204
15.3 Maxwell's Equations as a Hamiltonian System 205
15.4 Quantization of the Klein-Gordon and Maxwell Equations 207
15.4.1 The Quantization Procedure 208
15.4.2 Creation and Annihilation Operators 212
15.4.3 Wick Ordering 214
15.4.4 Quantizing Maxwell's Equations 215
15.5 Fock Space 216
15.6 Generalized Free Theory 219
15.7 Interactions 220
15.8 Quadratic Approximation 222
15.8.1 Further Discussion 228
15.8.2 A Brief Remark on Many-body Hamiltonians in Second Quantization and the Hartree Approximation 229

16 Quantum Electrodynamics of Non-relativistic Particles: The Theory of Radiation 231
16.1 The Hamiltonian 231
16.2 Perturbation Set-up 234
16.3 Results 236
16.4 Mathematical Supplements 239
16.4.1 Spectral Projections 239
16.4.2 Projecting-out Procedure 240

17 Supplement: Renormalization Group 241
17.1 The Decimation Map 242
17.2 Relative Bounds 243
17.3 Elimination of Particle and High Photon Energy Degrees of Freedom 244
17.4 Generalized Normal Form of Operators on Fock Space 248
17.5 The Hamiltonian $H_0(\varepsilon, z)$ 250
17.6 A Banach Space of Operators 254
17.7 Rescaling 255
17.8 The Renormalization Map 257
17.9 Linearized Flow 258
17.10 Central-stable Manifold for RG and Spectra of Hamiltonians 261
17.11 Appendix 265

18 Comments on Missing Topics, Literature, and Further Reading 267

References 273

Index 281

1

Physical Background

In this introductory chapter, we present a very brief overview of the basic structure of quantum mechanics, and touch on the physical motivation for the theory. A detailed mathematical discussion of quantum mechanics is the focus of the subsequent chapters.

1.1 The Double-Slit Experiment

Suppose a stream of electrons is fired at a shield in which two narrow slits have been cut (see Fig. 1.1.) On the other side of the shield is a detector screen.

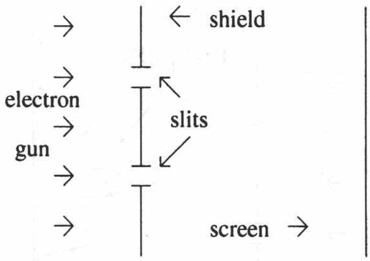

Fig. 1.1. Experimental set-up.

Each electron that passes through the shield hits the detector screen at some point, and these points of contact are recorded. Pictured in Fig. 1.2 and Fig. 1.3 are the intensity distributions observed on the screen when either of the slits is blocked.

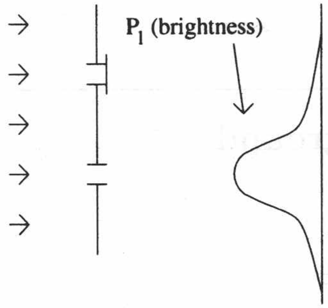

Fig. 1.2. First slit blocked.

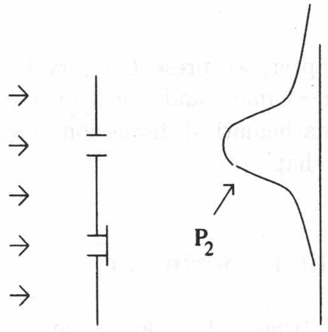

Fig. 1.3. Second slit blocked.

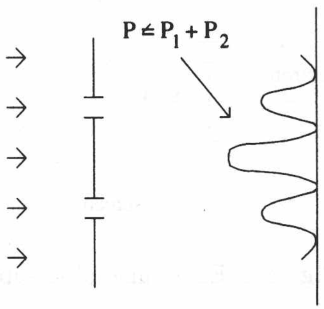

Fig. 1.4. Both slits open.

When both slits are open, the observed intensity distribution is shown in Fig. 1.4.

Remarkably, this is not the sum of the previous two distributions; i.e., $P \neq P_1 + P_2$. We make some observations based on this experiment.

1. We cannot predict exactly where a given electron will hit the screen, we can only determine the distribution of locations.

2. The intensity pattern (called an *interference pattern*) we observe when both slits are open is similar to the pattern we see when a wave propagates through the slits: the intensity observed when waves E_1 and E_2 (the waves here are represented by complex numbers encoding the amplitude and phase) originating at each slit are combined is proportional to $|E_1+E_2|^2 \neq |E_1|^2 + |E_2|^2$ (see Fig. 1.5).

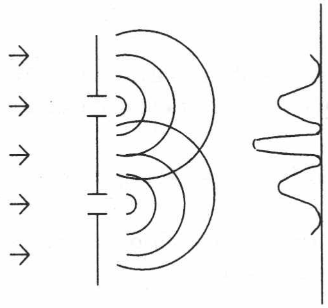

Fig.1.5. Wave interference.

We can draw some conclusions based on these observations.

1. Matter behaves in a random way.
2. Matter exhibits wave-like properties.

In other words, the behaviour of individual electrons is intrinsically random, and this randomness propagates according to laws of wave mechanics. These observations form a central part of the paradigm shift introduced by the theory of quantum mechanics.

1.2 Wave Functions

In quantum mechanics, the state of a particle is described by a complex-valued function of position and time, $\psi(x,t)$, $x \in \mathbb{R}^3$, $t \in \mathbb{R}$. This is called a *wave function* (or *state vector*). Here $\mathbb{R}^d$ denotes d-dimensional Euclidean space, $\mathbb{R} = \mathbb{R}^1$, and a vector $x \in \mathbb{R}^d$ can be written in coordinates as $x = (x_1, \ldots, x_d)$ with $x_j \in \mathbb{R}$.

In light of the above discussion, the wave function should have the following properties.

1. $|\psi(\cdot,t)|^2$ is the probability distribution for the particle's position. That is, the probability that a particle is in the region $\Omega \subset \mathbb{R}^3$ at time t is $\int_\Omega |\psi(x,t)|^2 dx$. Thus we require the normalization $\int_{\mathbb{R}^3} |\psi(x,t)|^2 dx = 1$.
2. ψ satisfies some sort of wave equation.

For example, in the double-slit experiment, if ψ_1 gives the state beyond the shield with the first slit closed, and ψ_2 gives the state beyond the shield with the second slit closed, then $\psi = \psi_1 + \psi_2$ describes the state with both slits open. The interference pattern observed in the latter case reflects the fact that $|\psi|^2 \neq |\psi_1|^2 + |\psi_2|^2$.

1.3 State Space

The space of all possible states of the particle at a given time is called the *state space.* For us, the state space of a particle will usually be the square-integrable functions:

$$L^2(\mathbb{R}^3) := \{\psi : \mathbb{R}^3 \to \mathbb{C} \mid \int_{\mathbb{R}^3} |\psi(x)|^2 dx < \infty\}$$

(we can impose the normalization condition as needed). This is a vector space, and has an inner-product given by

$$\langle \psi, \phi \rangle := \int_{\mathbb{R}^3} \bar{\psi}(x)\phi(x)dx$$

(in fact, it is a "Hilbert space" – see Section 1.5)

1.4 The Schrödinger Equation

We now give a motivation for the equation which governs the evolution of a particle's wave function. This is the celebrated *Schrödinger equation.*

Our equation should satisfy certain physically sensible properties.

1. The state $\psi(\cdot, t_0)$ at time $t = t_0$ should determine the state $\psi(\cdot, t)$ for all later times $t > t_0$ (*causality*).
2. If ψ and ϕ are evolutions of states, then $\alpha\psi + \beta\phi$ (α, β constants) should also describe the evolution of a state (the *superposition principle*).
3. In "everyday situations," quantum mechanics should be close to the classical mechanics we are used to (the *correspondence principle*).

The first requirement means that ψ should satisfy an equation which is first-order in time, namely

$$\frac{\partial}{\partial t}\psi = A\psi \tag{1.1}$$

for some operator A, acting on the state space. The second requirement implies that A must be a *linear* operator.

We use the third requirement in order to find the correct form of A. We first recall that one of the fundamental equations of classical mechanics is first-order in time. It is the *Hamilton-Jacobi equation,*

$$\frac{\partial}{\partial t}S = -h(x, \nabla_x S) \tag{1.2}$$

where $h(x,k) = \frac{|k|^2}{2m} + V(x)$ is the classical *Hamiltonian function*, V is the *potential*, m is the mass, and $S(x,t)$ is the classical *action*. This equation, in turn, is similar to the *eikonal equation*,

$$(\frac{\partial \phi}{\partial t})^2 - |\nabla_x \phi|^2 = 0$$

which is a high-frequency approximation of the wave equation for $u = ae^{i\phi}$. We make an analogy between the passage from the wave equation to the eikonal equation (that is, from *wave optics* to *geometric optics*) and the passage from quantum mechanics to classical mechanics. Thus, we require that Equation (1.1) (whose form we are seeking) has solutions of the form

$$\psi(x,t) = a(x,t)e^{iS(x,t)/\hbar}$$

where $\hbar$ is some very small constant, with S satisfying equation (1.2). Assuming a, S, and their derivatives are of order one in $\hbar$, then to the leading order in $\hbar$, ψ satisfies the equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\Delta_x\psi(x,t) + V(x)\psi(x,t). \tag{1.3}$$

The operator $\Delta = \sum_{j=1}^3 \partial_j^2$ is the *Laplacian* (in spatial dimension 3). This equation is of the desired form (1.1). In fact it is the correct equation, and is called the *Schrödinger equation*. It can be written as

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi = H\psi} \tag{1.4}$$

where the linear operator H, given by

$$\boxed{H\psi := -\frac{\hbar^2}{2m}\Delta\psi + V\psi}$$

is called a *Schrödinger operator*.

The small constant $\hbar$ is *Planck's constant*; it is one of the fundamental constants in nature. For the record, its value is roughly

$$\hbar \approx 6.6255 \times 10^{-27} \text{ erg sec.}$$

Example 1.1 Here are just a few examples of potentials.

1. Free motion : $V \equiv 0$.
2. A wall: $V \equiv 0$ on one side, $V \equiv \infty$ on the other (meaning $\psi \equiv 0$ here).
3. The double-slit experiment: $V \equiv \infty$ on the shield, and $V \equiv 0$ elsewhere.
4. The Coulomb potential : $V(x) = -\alpha/|x|$ (describes a hydrogen atom).
5. The harmonic oscillator : $V(x) = \frac{m\omega^2}{2}|x|^2$.

We will analyze some of these examples, and others, in Chapter 7.