

The Principles of Quantum Mechanics

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Preface

The premise of this book is that the principles of classical physics should follow from a correct and complete mathematics of quantum mechanics. The opposite approach has been taken since the origin of the “new” quantum mechanics in the 1920s, by discussing quantum mechanics as if it could be derived from classical physics. This has resulted in many issues of interpretation, and convoluted and incorrect mathematics. By applying the revised mathematics of quantum mechanics that I present in this book, it is possible to resolve some of the long standing issues in the field of quantum mechanics. As an example, the procedure of renormalization in quantum field theory can be given a precise meaning.

The ideas in this book evolved over forty years of physics education and practice, and that journey is summarized below. In college, I enjoyed a wonderfully coherent education on classical physics. The team of professors in physics, chemistry and mathematics coordinated a curriculum that aligned physics concepts with mathematical foundations and methods. This enabled me to see the beauty, elegance, and coherence of classical physics.

When I was introduced to quantum mechanics, I was disappointed by the way quantum concepts such as the probability rule, the complementarity principle, particle-wave duality, and the uncertainty principle are disconnected from the mathematics of quantum mechanics. It appeared there was a big gap in maturity, elegance, coherence and consistency between quantum mechanics and classical physics. I learned that others felt that way and that there had been an ongoing debate about this since quantum mechanics was formulated in 1926 (Jammer, 1966). That debate continues to this day (Wallace, 2008). I felt a need for a theory for quantum phenomena that achieved the same coherence and consistency as the classical theories I admired.

The existence of infinities in the theory of quantum fields was a known issue with quantum mechanics from the very beginning. Arcane computations are needed to extract finite numbers from formulas that lead to infinite results. These intricate spells and incantations first are invoked to regularize integrals, and then to “renormalize” parameters in the dynamical equations. While this has been accepted as a pragmatic solution because these manipulations do achieve miraculous agreement with experimental results, it is widely recognized that this is a problem.

In the summer of 1980, while working on my doctorate, I read “Integration in Hilbert Space” written by Skorohod (1974). It taught me the theory of measures on function spaces, not in the widely known context of probability theory and stochastic analysis, but as a basic part of functional analysis. Just as functional analysis appeared to me to be the mathematical foundation for quantum mechanics of systems with a finite number of degrees of freedom, this suggested one could formulate quantum mechanics of fields, which are infinite systems, as a natural generalization. The idea seemed so obvious that I was convinced that someone would quickly formulate an integrated theory of finite and infinite quantum systems.

As a computational scientist, much of my work was creating software that modeled

molecular reactions. I learned a method of using computers and computation as part of exploring abstract mathematical concepts, which I applied during the preparation of this book.

Over the years, I stayed informed about the developments in mathematics and in the foundations of quantum mechanics. I never saw the theoretical development that I expected from the application of functional analysis take place. This was confirmed when I sat in on a course on functional integration methods taught in the spring of 2004 by John Klauder. I decided to attempt to put together this theoretical development.

I started by gaining an understanding of functionals (functions of functions). This knowledge shed a new light for me on some of the unresolved issues in quantum field theory. I found that functionals are counterintuitive in a number of important ways. This insight provided the foundation for developing the ideas in this book, and further enabled me to carry out the required computations.

I consider what I am presenting to be a thorough revision of the principles of quantum mechanics, a revised edition as it were of the book by Dirac (1930) with the same title. There are two major areas of revision which are highlighted below.

In contrast to the traditional way of presenting quantum mechanics, I start from the premise that quantum mechanics is a theory of wave functions and of the dynamical law, the Heisenberg-Schrödinger-Dirac equation, that governs them as formulated in 1926. I do not start with quantum concepts such as the probability rule, the complementarity principle, particle-wave duality, and the uncertainty principle; instead, these are presented as derived concepts, obtained after a very lengthy and complicated mathematical journey.

Based on the work I did with functionals, I do not define interacting quantum fields by perturbation theory. Rather, quantum fields are defined as dynamical systems of quantum excitations, that have an internal structure produced by unavoidable self interaction. The methods known from and tested in nonrelativistic quantum mechanics can be generalized to apply to quantum fields. Perturbation theory can then be used to compute properties of quantum fields in ways that do not lead to Feynman diagrams with infinite integrals that must be regularized. The process of renormalization becomes a well-defined mathematical process that defines a new Hamiltonian operator, not just new parameters.

The revised principles open up new approaches to several open problems. For example, defining quantum fields with perturbation theory has obstructed a complete formulation of quantum chromodynamics and quantum gravity. The Yang-Mills quantum field theory can now be defined and used to formulate a theory of quantum chromodynamics with the property of asymptotic freedom and confinement. Similarly, a quantum theory for the dynamics of space and the effects of gravity can be formulated.

The book is organized into three parts:

1. The first part introduces the physics concepts and explains how they work together to make a consistent theory. The first chapter “Principles” gives an overview and the remaining chapters provide the details. The first part is intended primarily for physicists.
2. The second part applies the principles from the first part to give the quantum theory of electrons and photons, of quarks and gluons, and of the geometry of space.

3. The third part is for the reader who seeks precision and rigor. It provides the mathematical and computational details. This part has a number of chapters with reference material as well as derivations and proofs to provide the foundation for the results obtained in the first part. The third part is intended primarily for mathematicians, and the format reflects that.

Links and cross references between the parts should allow the reader to start with the first part, learn things from the third part as the need arises, and then read the application of the principles in the second part.

The reader may wish to leaf through the book at first, reading only the short “trail markers”. They give a brief overview of what happens close to the marker and provide guidance on how the complete story hangs together. The location of every trail marker can be found in the Index under “trail marker.”

I hope the reader will enjoy the exploration of the consequences that have been opened up by these updated principles of quantum mechanics as much as I did.

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Gainesville, Florida
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I want to thank my publisher Sonke Adlung. We met in 2004 to talk about the book. He encouraged me throughout the decade-long period to develop and write the book.

Above all I feel lucky to have found my wife Liz. I am thankful to her and our children, Eleanor and Edward, for their love and support. They were stuck with me through this long journey and put up with my drive to understand quantum mechanics and then to write it all down. I also thank her for the proofreading she did of the whole book skillfully navigating the math she is not familiar with to give meaningful and valuable feedback on the writing and the consistency and coherence of the story.

Contents

PART I FOUNDATION

1 Principles	3
1.1 Terminology	4
1.1.1 Kinematics	4
1.1.2 Dynamics	5
1.1.3 Mechanics	5
1.1.4 Statistics	5
1.1.5 Measurement	6
1.2 Dynamical law	7
1.3 Phase space	8
1.4 System specification and entanglement	10
1.5 Natural degrees of freedom	11
1.6 Natural systems	13
1.7 Classical systems	14
1.8 Experimental observation	16
1.9 Summary	18
2 Finite quantum systems	21
2.1 Kinematics	22
2.1.1 Phase space and state	23
2.1.2 Characteristics and spectral representation functions (srf)	24
2.1.3 Free motion	26
2.2 Dynamics	28
2.2.1 Oscillator	29
2.2.2 Entanglement	32
2.2.3 Phase space for composite systems	33
2.2.4 Dynamics of composite quantum systems	35
2.2.5 Coulomb systems	39
2.3 Rayleigh-Schrödinger perturbation theory	41
2.3.1 Convergent and asymptotic series	45
2.3.2 Secular perturbation theory	46
2.4 Mean field theory	48
2.5 Born-Oppenheimer theory	50
2.6 Different pictures of phase space	52
2.6.1 Heisenberg picture	52
2.6.2 Schrödinger picture	53
2.6.3 Feynman picture	53
2.6.4 Path integrals	55
3 Relativistic quantum fields	59

3.1	Why only fields?	60
3.2	Kinematics	62
3.2.1	Classical theory of fields	62
3.2.2	Configuration space and phase space	67
3.2.3	Intuitive view of infinity	68
3.2.4	Gaussian measure	72
3.2.5	Definition of quantum fields	74
3.3	Wightman picture	77
3.3.1	Spacetime symmetry groups	79
3.3.2	Euclidean group representation	81
3.3.3	Time translations and Lorentz boosts	82
3.3.4	Spatial momentum operators	83
3.3.5	Reducible and decomposable representations	85
3.4	Free scalar field	86
3.4.1	Field momentum operator	87
3.4.2	Hamiltonian operator	88
3.4.3	Quantum field wave functionals	92
3.4.4	Poincaré group representation	96
3.4.5	Field operators	98
3.5	Dynamics	99
3.5.1	Spectral analysis	101
3.5.2	Self interaction	103
3.5.3	Quantum field with explicit vacuum	104
3.5.4	Quantum field with φ^4 potential	105
3.5.5	Composition of quantum fields	107
3.6	Generalized free scalar field	108
3.6.1	Separation of $\tilde{\varphi}^4$ mode variables	110
3.6.2	Vacuum wave functional	114
3.6.3	One-quantum wave functionals	115
3.6.4	Spectrum of the Poincaré-group representation	115
3.6.5	Phase space structure	118
3.6.6	Generalized-free-field operators	120
3.7	Scalar field with φ^4 potential	121
3.7.1	Mean field theory	121
3.7.2	Spectral transformation kernels	123
3.7.3	Asymptotic wave functionals for collision processes	125
3.7.4	Perturbation theory	129
4	Macroscopic quantum systems	135
4.1	Classical mechanics	137
4.1.1	Dynamical state and phase space	137
4.1.2	Dynamical law and phase-space flow	138
4.1.3	Characteristics	138
4.1.4	Composite systems	139
4.1.5	No intrinsic scale	139
4.1.6	Statistical state	140
4.1.7	Observables	141

4.1.8	Summary	141
4.2	Quantum mechanics	141
4.2.1	Dynamical state and phase space	142
4.2.2	Dynamical law and phase-space flow	143
4.2.3	Characteristics	144
4.2.4	Composite systems	147
4.2.5	Natural scales	149
4.2.6	Statistical state	150
4.2.7	Summary	151
4.3	Classical systems and measurement	152
4.3.1	Values from functions	153
4.3.2	Probability	156
4.3.3	Born-von-Neumann rule	157
4.3.4	Two-slit interference experiment	158
4.4	On interpretation	162
PART II THEORY OF MATTER AND FORCES		
5	Principles of gauge theory	167
5.1	Matter equations	169
5.2	Global gauge transformations	170
5.2.1	Abelian gauge group $U(1)$	170
5.2.2	Non-Abelian gauge group $SU(3)$	171
5.3	Maxwell equations	173
5.4	Yang-Mills equations	175
5.5	Local gauge transformations	179
5.5.1	Abelian local gauge transformations	179
5.5.2	Non-Abelian local gauge transformations	180
5.6	Coupled matter and gauge potential equations	182
5.7	Dynamics of gauge potentials	183
5.7.1	Gauge constraints	183
5.7.2	Equivalence classes of gauge evolution	187
5.8	Mathematical formulation of gauge theory	189
5.8.1	Manifolds and fiber bundles	189
5.8.2	Infinite-dimensional Lie groups	190
6	Quantum electrodynamics	193
6.1	Free fields	195
6.1.1	Classical spinor dynamics	195
6.1.2	Real Majorana spin waves	199
6.1.3	Configuration space and phase space	201
6.1.4	Fock space representation	202
6.2	Heisenberg, Wightman, and Weyl pictures	203
6.2.1	Spacetime symmetry	204
6.2.2	Constraints in quantum mechanics	206
6.2.3	Gauge conditions	206
6.2.4	Gauge theory of quantum fields	207
6.3	Structure from dynamics	209

6.3.1	Interaction terms	210
6.3.2	Spectral representation	211
6.3.3	Spacetime representation	213
6.3.4	Building the electron	215
6.3.5	Effective field theory	219
7	Quantum chromodynamics	221
7.1	Confinement and asymptotic freedom	222
7.2	Kinematics	224
7.2.1	Configuration space	224
7.2.2	Phase space	226
7.2.3	Free matter and potential fields	227
7.2.4	Spectral representation	229
7.2.5	Wightman and Weyl pictures	231
7.2.6	Charges and conserved currents	235
7.2.7	Field coordinates	236
7.3	Confinement from dynamics	238
7.3.1	Building chroma-neutral excitations	239
7.3.2	Fractional electric charge	241
8	Quantum geometrodynamics	243
8.1	Recapitulation of general relativity	244
8.2	The principle of local symmetry	248
8.3	Kinematics	252
8.3.1	Spacetime coordinates	252
8.3.2	Configuration space	253
8.3.3	Phase space	254
8.3.4	Schödinger equation	255
8.3.5	Static spacetime	256
8.4	Dynamics	256
8.4.1	Dynamic spacetime	257
8.4.2	Space and matter	258
8.4.3	Black holes	259
PART III MATHEMATICS		
9	Mathematics primer	263
9.1	Computation	263
9.2	Hilbert spaces	264
9.2.1	Analysis of the sphere	265
9.2.2	Dense subspaces	270
9.3	Measure theory	272
9.3.1	Orthogonal and unitary transformations	274
9.4	Example with Brownian motion paths	275
9.4.1	Brownian Bridge measure	275
9.4.2	Brownian Bridge density in position space	277
9.4.3	Wiener measure	279
9.4.4	Wiener density in position space	282

9.4.5	Doubly mixed measure	282
9.4.6	Visualization	283
9.4.7	Interior and surface	284
9.5	Integrals	285
9.6	Manifolds and groups	286
10	Path integrals	289
10.1	Time slicing	289
10.2	Feynman ε -regularization	292
10.2.1	Heat kernel	293
10.2.2	Schrödinger kernel	294
10.2.3	Brownian motion paths	295
10.2.4	Lagrangian motion paths	299
10.2.5	The limit $\varepsilon \rightarrow 0$	301
10.3	Functional analysis of time slicing	303
10.4	The square-well potential	307
10.5	Relativistic path spaces	308
10.5.1	Velocity paths	309
10.5.2	Rapidity paths	310
10.6	Numerical evaluation of path integrals	312
10.7	Sheet integrals	314
10.8	$(d + 1)$ -path integrals	317
11	Kinematics of quantum systems	321
11.1	Theory of mechanics	321
11.2	Configuration space	323
11.2.1	Gaussian measure	323
11.2.2	Symmetry of physical space	325
11.2.3	Cylinder approximation	328
11.3	Phase space	331
11.3.1	Special role of polynomials	332
11.3.2	Spacetime symmetry	333
11.4	Basic operators	334
11.4.1	Multiplicative operator	334
11.4.2	Gradient operator	336
11.4.3	Fourier-Gauss transform	339
11.4.4	Laplace operator	347
11.5	Representation of the rotation and Euclidean groups	351
11.5.1	Scalar representation	352
11.5.2	Spinor representation	355
11.6	Force-constant operators	356
11.7	Spherical oscillator $\Delta \parallel A_1$	359
11.7.1	Creation and annihilation operators	361
11.7.2	Polynomial Fock basis	363
12	Dynamics of quantum systems	367
12.1	Confined field oscillator $\Delta \parallel A_2$	368
12.1.1	Aligned Fock basis	374

12.1.2	On wave functionals and measures	379
12.2	Free field oscillator Δ, A_3 not aligned	380
12.2.1	Canonical view	386
12.3	Free field evolution	388
12.4	Potential functionals	391
12.4.1	Special sextic polynomial	393
12.4.2	Quartic polynomial	396
12.5	Scalar field Hamiltonian $\Delta \parallel A_2 \parallel V_1$	402
12.6	φ^4 field Hamiltonian Δ, A_3 , and V_2 not aligned	406
12.7	Representation of the Lorentz and Poincaré groups	409
12.7.1	Time translations	409
12.7.2	Boosts	410
12.7.3	Spinor representation	412
12.7.4	Canonical representation in Fock space	412
12.7.5	Casimir operators	414
12.8	Operator valued equations	418
12.9	Numerical construction of spectral representation	419
13	Informatics of quantum systems	423
13.1	Information theory	424
13.1.1	Data collection	424
13.1.2	Data modeling	426
13.1.3	Validation and uncertainty quantification	428
13.1.4	Physics	428
13.2	Classical mechanics	430
13.2.1	Dynamical law	430
13.2.2	Probability	431
13.3	Quantum mechanics	434
13.3.1	Dynamical law	434
13.3.2	Composite systems	437
13.3.3	Probability	441
13.4	Classical from quantum	442
13.4.1	Values	442
13.4.2	Randomness	444
13.4.3	Information	445
Appendix A	Hilbert spaces	451
A.1	Definitions and axioms	451
A.2	Spectral analysis	454
A.3	Fock space	460
Appendix B	Measure theory	463
B.1	Finite-dimensional spaces	463
B.2	Infinite-dimensional spaces	468
B.2.1	No measure like Lebesgue measure	468
B.2.2	Cylinder sets	469
B.2.3	Finite measures	470
B.2.4	Cameron-Martin space	474

B.2.5	Mixed measures	479
B.2.6	Measurable linear and polynomial functionals	480
B.3	Smoothness of paths	483
B.4	Measure space of absolutely continuous paths	485
B.5	Local characterization	489
Appendix C	Manifolds and groups	491
C.1	Differentiable manifolds	491
C.1.1	Topology	491
C.1.2	Charts	493
C.1.3	Vectors, one-forms, and tensors	494
C.1.4	Derivative and pullback of a smooth map	495
C.2	Lie groups	496
C.2.1	Group theory	496
C.2.2	Classical matrix groups	498
C.2.3	Lie algebras	502
C.2.4	Normed group algebras	507
C.3	Fiber bundles	508
C.3.1	Lie group action	510
C.4	Connection and curvature	512
C.5	Coordinatization	514
C.6	Infinite-dimensional Lie groups	515
References		517
Index		537

List of figures

3.1	Lorentz boost for fields	82
3.2	Wightman picture	84
3.3	Spectral sheets with continuous-spectrum force-constant operator	96
3.4	Spectrum of free-field Poincaré group representation	98
3.5	Sextic potential eigenfunctions	105
3.6	$\tilde{\varphi}^4$ mode wave functions	113
3.7	Spectrum of $\tilde{\varphi}^4$ Poincaré group representation	116
4.1	Diffraction pattern	146
4.2	Quantum to classical	155
4.3	Two-slit experiment	159
4.4	Biprism geometry	159
8.1	Static spacetime geometry	256
8.2	Dynamic spacetime geometry	258
9.1	Segments and wedges	266
9.2	Brownian Bridge kernel	278
9.3	Brownian Bridge and Wiener position density widths	280
9.4	Cameron-Martin ellipsoid	283
11.1	Cylinder approximation	329
11.2	Defining operators	333
12.1	Spectral sheets with discrete-spectrum force-constant operator	374
12.2	Flowchart of φ^4 spectral analysis	392
12.3	Sextic potential eigenfunctions structure	395
12.4	Sextic potentials for different modes	396
12.5	Construction of interacting field theory	401

List of tables

8.1	Theory lineup	249
8.2	Field lineup	250
9.1	Edges of a wedge	268
10.1	Trace of covariance $(-\Delta)^{-p}$	320
11.1	Trace of covariance Γ	325
11.2	Enumeration of Fock basis $(\Phi_\mu)_\mu$	365
12.1	Fock space dimension	419
12.2	Maple TM procedures	420

Notation

In general the meaning of symbols is made clear in the immediate context of where the symbol is used, section or theorem. However, there are a number of symbols that have a consistent meaning throughout the book. These definitions are collected here for convenience.

Sets and spaces. The set of natural numbers $1, 2, 3, \dots$ is denoted \mathbb{N} , the set of all integers $\{0, \pm 1, \pm 2, \pm 3, \dots\}$ by \mathbb{Z} , and the set of rational numbers $\{n/m | n, m \in \mathbb{Z}, m \neq 0\}$ by \mathbb{Q} . The real numbers are \mathbb{R} and the complex numbers \mathbb{C} .

The topological dual of a topological space X is the space of continuous linear functionals on that space and is denoted by X^* .

The physical space we live in is denoted in general by \mathbb{R}^d , where the dimension of space d is 3, but can be 1 or 2, or even larger than 3. The dimension of spacetime is then $d + 1$.

The convention for spacetime is to put spatial coordinates first $r = (\vec{r}, t)$ with positive signature in the metric

$$\eta = g = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$$

so that the Minkowski product is

$$a_i b^i = \eta_{ij} a^j b^i = \sum_{i,j=1}^4 \eta_{ij} a^j b^i = a^1 b^1 + a^2 b^2 + a^3 b^3 - a^4 b^4.$$

The notation for measurable square-integrable functions on a space X with a measure μ taking values in a space Y is denoted in the literature as $L^2(X, \mu, Y)$ or as $L^2(X, Y, \mu)$. When the measure is the Lebesgue measure λ , it is often omitted, so the notation becomes $L^2(X, Y)$. When the functions are real- or complex-valued, $Y = (\mathbb{R})$ or \mathbb{C} , the Hilbert space is written simply as $L^2(X)$.

The Hilbert space of real field configurations φ on space is denoted $\mathbb{F} = L^2(\mathbb{R}^d, \lambda, \mathbb{R}) = L^2(\mathbb{R}^d)$, with the last equality as a shorter specification; λ denotes the Lebesgue measure on \mathbb{R}^d ; the final argument denotes the target space of the functions.

The Hilbert space of complex wave functionals Φ of fields is $\mathbb{H} = L^2(\mathbb{F}, \gamma, \mathbb{C})$, where γ is a measure on \mathbb{F} .

The Fock space generated with a Hilbert space X is denoted by $\mathcal{F}(X)$.

The standard Lie groups are denoted with capital letters: $SO(3), SU(2), SO(3, 1)$. The universal covering group is denoted with a line over the entire name: $\overline{SO(3)}$. The Lie algebra of the group is denoted with lowercase letters: $so(3), su(2), so(3, 1)$. The infinite-dimensional Lie group that is the local gauge group obtained by allowing gauge transformations change with location in space is denoted by putting a script letter “ ℓ ” in front of

the name of the global gauge group: $\ell SU(3)$; The corresponding infinite-dimensional Lie algebra is denoted $\ell su(3)$.

Elements. An array of numbers is denoted with a bar over the symbol: $\bar{x} = (x_1, \dots, x_n)$.

A possibly infinite vector $\bar{\mu} = (\mu_1, \mu_2, \dots)$ with each entry $\mu_m = 0, 1, 2, \dots$ an index of some kind is called a *multi-index*.

The norm of the multi-index μ is given by $|\bar{\mu}| = \sum_{m=1}^{\infty} \mu_m$.

Let $\bar{\varepsilon}_m = (0, \dots, 0, 1, 0, \dots)$ denote the multi-index with only the index 1 at location m . Then the multi-indices $\bar{\mu} = (\mu_1, \dots, \mu_{m-1}, \mu_m \pm 1, \mu_{m+1}, \dots)$ can be written as $\bar{\mu} \pm \bar{\varepsilon}_m$.

When the meaning is clear from the context, we often omit the bar over the multi-index symbol to simplify notation. The norm of a multi-index gives the total number of excitations for one type of multi-index that we will use.

The set \mathbb{K} of values of the multi-index ν is not totally ordered.

We use Roman letters for position in space and time. Vectors in d -dimensional physical space are denoted with the arrow over the symbol: $\vec{x} = \sum_i x_i \vec{e}_i$.

An element of a Lie algebra with generators T_1, \dots, T_n and coefficients $\bar{\omega} = (\omega_1, \dots, \omega_n)$ is denoted with a box superscript as $\omega^\square = \sum_a \omega_a T_a$. To be consistent, one should put the box superscript on the generators of the algebra; but there is no such practice in the literature, so we will not do that either.

Vectors and matrices in general linear spaces like \mathbb{R}^N and \mathbb{C}^N are denoted in boldface.

Fields in space in general are denoted by lowercase Greek letters $\varphi(\vec{x})$. The time evolution of a field is then a function from the real axis of time \mathbb{R} into \mathbb{F} and can be written as $\varphi(t)$, φ_t , or $\varphi(\vec{x}, t)$ depending on the context.

wave functions of finite systems and wave functionals of infinite systems and fields are denoted by capital Greek letters $\Psi(x)$ and $\Psi[\varphi]$, respectively. The Dirac notation for elements of the Hilbert space \mathbb{H} is the bra-ket notation $|\alpha\rangle$. The wave function is then $\Psi(x) = \langle x | \Psi \rangle$.

Linear operators in \mathbb{H} are in bold, those in \mathbb{F} are in regular typeface, possibly with a hat.

An \mathbb{F} -vector-valued linear operator in \mathbb{H} is denoted by a bold symbol with a bar over it, when it is desirable to clearly exhibit the vector nature of the result of the operator.

The Kronecker delta is $\delta_{kl} = 1$ for $k = l$ and zero otherwise for k and l integer.

The Levi-Civita or permutation symbol is defined as

$$\varepsilon_{ijk} = \begin{cases} 1 & (i, j, k) = \text{cyclic}(1, 2, 3) \\ -1 & (i, j, k) = \text{cyclic}(1, 3, 2) \\ 0 & \text{otherwise} \end{cases}$$

The three complex 2×2 matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are called the Pauli matrices. They are a basis for the Lie algebra of the Lie group $SU(2)$.

The 4×4 Dirac matrices (Thaller, 1992, p. 36) have a representation with real matrix elements introduced by Majorana (1937)

$$\alpha_1 = \begin{pmatrix} \sigma_1 & 0 \\ 0 & -\sigma_1 \end{pmatrix} \quad \alpha_2 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \quad \alpha_3 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix} \quad \beta' = -i\beta = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

xx Notation

In that representation the gamma matrices $\gamma^j = -\beta^j \alpha_j, j = 1, 2, 3$ and $\gamma^4 = -\beta^4$ become

$$\gamma^1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix} \quad \gamma^2 = \begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix} \quad \gamma^3 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix} \quad \gamma^4 = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}.$$

Writing the contraction of a four-vector and the gamma matrices $\sum_{\nu=1}^4 p^\nu \gamma^\nu = \not{p}$ as 4×4 spinor matrix is known as the Feynman slash notation.

The Gell-Mann matrices λ_j are the eight complex 3×3 matrices (Burgess and Moore, 2007, p. 44) given by

$$\begin{aligned} \lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \lambda_2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \lambda_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \lambda_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} & \lambda_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} & \lambda_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\ \lambda_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} & \lambda_8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \end{aligned}$$

They are a basis for the Lie algebra of the Lie group $SU(2)$.

Operations. The composition of functions is denoted by \circ , which means that $(f \circ g)(x) = f(g(x))$.

The time derivative of a function or field is sometimes denoted by a dot over the symbol: \dot{f} .

The symbol \circ is also used to denote an abstract group composition law in chapter C.

The wedge product of two one-forms is denoted $\omega \wedge \omega$.

Complex conjugation is denoted by the asterisk superscript: a^* .

The Fourier transform of a function f is denoted by $\mathcal{F}f = \tilde{f}$ and is defined as

$$\tilde{f}(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{iyx} f(x) dx$$

The adjoint of an operator is denoted by the dagger superscript: A^\dagger .

In physics the convention is to place the complex conjugation on the first element in the scalar product, whereas the mathematical literature usually places the conjugation on the second element. We use the physics convention.

A multi-index $\bar{\alpha}$ is an array $(\alpha_1, \dots, \alpha_m)$ of positive integers. The sum of the components is denoted $|\bar{\alpha}| = \alpha_1 + \dots + \alpha_m$. The partial derivative of a function f of m variables can then be written as

$$D^\alpha f = D_1^{\alpha_1} \dots D_m^{\alpha_m} f = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \dots \partial x_m^{\alpha_m}}$$

The integral of a function f with respect to a measure μ over a measurable set $A \subset X$ is written as

$$\int_A f d\mu = \int_A f(x) \mu(dx)$$

where the variable x takes on values in the space X .

Use of complex numbers. Complex numbers have many uses in quantum mechanics and these uses often overlap causing some confusion. Fortunately, this rarely leads to serious errors. We will keep the uses clearly separated.

1. Quantum mechanical wave functions and wave functionals are inherently complex because the Schrödinger equation has i in it explicitly. We will use complex valued wave functionals. They are elements of the Hilbert space \mathbb{H} .
2. Classical fields φ , like the scalar field considered in this chapter, are assumed to be real. The Hilbert space of field configurations \mathbb{F} is therefore real. When we use the Fourier transform, we use the sine-cosine form to map real functions to real functions.
3. Charged fields are often written as complex fields $\varphi = \varphi_1 + i\varphi_2$ with the gauge group $U(1)$. This would lead to loading double use on complex numbers. We will then use the two components (φ_1, φ_2) to build the Hilbert space \mathbb{F} of configurations.
4. Spin one-half fields are naturally described by two-component, complex fields associated with the universal covering group $SU(2)$ of $SO(3)$. This leads to another chance for double use of the complex numbers. The four-component Dirac field itself uses complex numbers twice already: Once to create a charged field that is the sum of two Majorana fields, which themselves already use complex numbers to create spin one-half fields. As a rule we will consider real Hilbert spaces \mathbb{F} with appropriate multi-component, real fields.

The complex numbers can be represented as real 2×2 matrices as follows

$$a + ib \longleftrightarrow \begin{pmatrix} a & -b \\ b & a \end{pmatrix},$$

such that matrix addition and multiplication correspond to addition and multiplication of complex numbers

$$\begin{aligned} (a + ib)(c + id) &= ac - bd + i(ad + bc) = u + iv \\ \longleftrightarrow \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \begin{pmatrix} c & -d \\ d & c \end{pmatrix} &= \begin{pmatrix} ac - bd & -ad - bc \\ bc + ad & -bd + ac \end{pmatrix} = \begin{pmatrix} u & -v \\ v & u \end{pmatrix}. \end{aligned}$$

This allows for quick transformation of any complex number into a real matrix form.

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Index

- *, xviii
- A^μ , 173, 176
- $C^\infty(X)$, 453
- $C_0^\infty(X)$, 453
- $D^{(m)}$, 363, 376, 415
- $F^{\mu\nu}$, 174, 176
- $H^m(X)$, 453
- $L^p(X)$, 452
- $SO(3)$, 504
- $SO^+(3, 1)$, 505
- $SU(2)$, xix, 504
- $SU(3)$, xx, 506
- $W^{m,p}(X)$, 453
- $Z^{(m)}$, 363, 376, 415
- superscript, xix, 172
- o, xx
- †, xx
- C, xviii
- F, 67, 331
- H, 67, 331, 335
- N, xviii
- Q, xviii
- R, xviii
- Z, xviii
- $\mathcal{F}^{\mu\nu}$, 176
- $\overline{\mathbb{H}}$, 335, 388
- ~, xx
- ^, xx
- ., 50

- a.e., 70, 466
- a.s., 466
- Abelian, 497
- Abraham-Lorentz, 61
- Abraham-Lorentz-Dirac, 61
- absolutely continuous, 299, 467, 483, 485
- action
 - free, 511
 - left, 510
 - right, 510
 - transitive, 511
- adiabatic, 50
- adjoint operator
 - notation for, xx
- admissible direction, 336–338, 347, 349, 358, 474
- algebra, 502
 - Clifford, 65, 195
 - derivation, 502
 - Lie, xviii, 287, 491
 - normed, 287, 507
- algorithm, 303, 308, 490

- aligned, 90, 356
- almost everywhere, 70, 466
- almost surely, 163, 466, 476
- antisymmetric symbol, 414
- associative, 496, 502
- asymptotic freedom, 222
- atlas, 286, 493, 508
 - compatible, 493
 - complete, 493
- atom, 40
 - hydrogen, 217
- Avogadro's number, 12, 72, 442

- basis
 - aligned Fock, 91, 101, 375, 402
 - Fock, 371
 - linear space, 451
 - polynomial Fock, 90, 364, 375
- Bianchi relations, 248
- bilinear, 499
- black box, 136
- Bohr radius, 145
- Borel summability, 47
- Born approximation
 - distorted wave, 133
- Born-Oppenheimer, 50, 216
- Born-von-Neumann rule, 17, 22, 157, 435, 439
- boundary condition
 - Dirichlet, 276, 281, 315
 - Neumann, 309
- Brownian Bridge, 277, 293, 483
 - stochastic process, 277
- Brownian motion path, 296
- bundle
 - associated, 512
 - cotangent, 509
 - fiber, 508, 511
 - frame, 512
 - horizontal, 509, 513
 - map, 509
 - morphism, 509
 - principal, 511, 512
 - section, 510
 - tangent, 509, 513
 - trivial, 508
 - vector, 509
 - vertical, 509, 513

- canonical commutation, 338
- canonical transformation, 139
- canonical view, 92, 104, 211, 328, 349, 356, 403
- Cantor enumeration, 364

- Cauchy data, 5
- Cauchy principal value, 44
- Cauchy problem, 5, 15, 29, 245, 315, 321, 429, 431, 435
- characteristic, 10, 24, 67, 74, 138, 141, 144, 151, 321, 436
- charge, 236
 - elementary, 145
- chart, 286, 493
- checkerboard, 308
- Christoffel symbol, 244
- chromodynamics, 506
- classical tip, 154, 157
- classical tip system, 444
- closure, 271
- cocycle condition, 512
- collision, 102, 126
- commutative, 223, 497
- compact, 265
- complementarity, 18
- complex conjugation
 - convention, xx
 - notation for, xx
- complex numbers
 - as 2×2 matrices, xxi
- complexification, 456
- composition, xx
- Compton wavelength, 62, 386
- concentration
 - cone of, 481
 - ellipsoid of, 298, 473
- configuration space, 274
- configurations, 323, 331
- confinement, 223
- connection, 190, 244, 509, 513
- constraint, 12, 36, 139, 183
 - forcing, 12, 206, 252
 - holonomic, 185, 197
 - nonholonomic, 185, 197, 207
 - symmetry, 12, 194, 203, 206, 252
- continuous, 492
- contravariant, 247, 493
 - vector, 494
- convex, 310
- convolution, 93
- coset, 497, 510
- Coulomb potential, 39, 184, 185, 212, 241
- covariance, 324, 331, 368
- covariant, 247, 493
 - vector, 494
- covariant derivative, 176, 179, 182, 190, 513, 515, 516
 - gauge, 177, 251
 - spacetime, 247, 251
- curvature, 162, 190, 514
 - extrinsic, 246
 - intrinsic, 246
- curvature tensor, 244
- curve, 494, 509, 513
- cylinder
 - base, 72, 237, 469
 - function, 403, 470
 - operator, 360, 370
 - set, 73, 299, 313, 469
 - vertical, 470
- d'Alembertian, 316
- de Broglie, 7, 158
- deep inelastic scattering, 221
- degree of freedom, 24, 137
- density
 - charge, 171
 - spinor length, 197, 198
- density of paths, 294
- derivative
 - Lie, 495
 - logarithmic, 336, 339, 353, 376, 387
 - map, 495
- differentiable manifold, 493, 508
- differential, 495
- differential equation
 - ordinary, 5
 - partial, 5
- differential geometry, 189, 286
- diffraction, 17
- dimension
 - Hausdorff, 466
 - Hilbert space, 271
 - linear space, 451
- Dirac matrices, xix, 64, 65, 195
- direct integral, 86
- dispersion, 410
- dispersion relation, 102, 117, 133
- distribution
 - generalized function, 74
 - Schwartz, 74
 - tempered Schwartz, 74
- dressed, 101
- dynamical law, 321, 429
- dynamics, 5, 10, 321
- Earth, 286
- Eichinvarianz, 168
- Einstein convention, 494
- electrodynamics, 60, 169
 - principal bundle, 516
- electron, 61, 193
- emergence of values, 154
- energy-momentum tensor, 244
- entanglement, 10, 11, 13, 14, 32, 154, 438, 440, 447
- equation
 - diffusion, 293
 - Dirac, 62, 195, 308
 - Einstein, 258
 - Fredholm, 276
 - geodesic, 244
 - Hamilton, 138
 - Hartree-Fock, 49
 - Hartree-Fock-Bogolubov, 123
 - heat, 293
 - Heun, 112, 396
 - hypergeometric, 112
 - Klein-Gordon, 62, 179, 314, 386, 389, 418

- Liouville, 140, 432
- Majorana, 62, 195, 199
- Maxwell, 173
- Newton, 138
- Schrödinger, 23, 204, 293
- wave, 314
- equivariant, 513
- excitation, 26, 417
- exclusion principle, 202
- exponential map, 170, 191, 505, 515
- Feynman slash, xx
- Feynman-Kac formula, 291
- fiber, 470, 509
- field
 - boost operator, 336
 - chroma, 168, 175, 221
 - color, 175, 221
 - electromagnetic, 5, 6, 168, 173
 - evolution of, 4
 - force, 168
 - Hilbert space, 86
 - matter, 168
 - momentum operator, 338
 - of Hilbert spaces, 508
 - operator, 335
 - potential, 173, 176
 - quantum, 460
 - strength, 174, 176, 514
 - velocity, 5
- flow, 427
 - Hamilton-Poincaré, 138, 431
 - Heisenberg-Schrödinger, 143, 435
 - time-dependent, 138
- foliation, 245
- force
 - electromagnetic, 168, 223
 - gravity, 168
 - nuclear, 168, 221
- Fourier transform, xx, 73, 91, 348, 368
 - real, 354
- Fourier-Gauss transform, 344
- frame, 511
- function
 - Borel, 463
 - cylinder, 237, 308, 313, 345, 403, 470
 - Green, 54, 145, 214, 290, 294, 316
 - Hermite, 30, 47, 226
 - index, 349
 - measurable, 299, 452, 463, 482
 - properly linear, 482
 - rapid decrease, 70
 - Schwartz, 70
 - simple, 466
 - with compact support, 453
- functional, 68
 - cylinder, 72
 - multi-linear, 482
- functional calculus, 383
- fundamental vector fields, 513
- G, 244
- Galilei boost, 409
- gamma matrices, xx
- gauge
 - Coulomb, 184
 - Lorenz, 184, 187
 - radiation, 184
 - transverse, 184
- gauge condition, 183, 514
- gauge group, 191, 515
 - global, 170, 506, 514
 - local, 191
 - spatially local, 191
- gauge potential, 176, 514
- gauge symmetry, 491
- gauge theory, 168, 223, 515
- gauge transformation, 179
- Gell-Mann matrices, xx, 172, 506
- generalized free field, 107, 110, 120, 133
- geodesic, 244
- Gibbs phenomenon, 282, 305, 480
- gluon, 223
- gravity, 162
- Green function, 214
- group, 286, 496
 - normal subgroup, 497
 - Abelian, 501
 - compact, 500
 - conjugate subgroup, 497
 - Euclidean, 79, 205, 286, 414, 500
 - factor, 497, 503
 - global gauge, xix
 - invariant subgroup, 497
 - left action, 510
 - Lie, xviii, 79, 287, 414, 491, 492, 496, 504, 511
 - local gauge, xviii
 - Lorentz, 80, 287
 - Poincaré, 75, 80, 205, 287, 414, 501
 - quotient, 497
 - representation, 287, 504
 - right action, 510
 - rotation, 64, 79, 205, 287
 - special orthogonal, 79
 - special unitary, 79
 - stability, 511
 - universal covering, xviii, 503
- Hölder continuous, 483
- Hamiltonian
 - φ^4 field, 109
 - electronic, 51
 - free field, 91
 - quantum chromodynamics, 228
 - quantum electrodynamics, 204
- harmonic
 - coordinates, 255
- Hartree-Fock, 48, 50
- Hartree-Fock method, 133
- helicity, 415
- Hermite polynomials, 30, 359, 370, 482
- Hermitian, 25
- Heun function, 396

- Heun identity, 397
- Hilbert-Schmidt operator, 306, 477
- homomorphism, 497

- index function, 44, 85, 92, 355, 357, 385
- inertial frame, 311
- informatics, 15, 322
- infraparticle, 106, 120, 121, 133
- initial-value problem, 29, 245, 321
- integral, 272
 - Feynman, 55
 - Feynman ε -regularized, 293
 - Feynman time-slicing, 290
 - Lebesgue, 466
 - notation, xx, 466
 - path, 55, 207
 - Riemann, 54, 466
- interpretation, 7
- intuition, 265
- ion, 40
- isomorphism, 497

- Källén-Lehmann representation, 86, 120, 413
- kinematics, 4, 10, 321
- Klein-Gordon equation, 208
- Kronecker delta, xix, 80, 352, 373, 409

- Lagrange multipliers, 185, 197
- Lagrangian, 311
- Lagrangian motion path, 299
- Laplace operator, 316, 347, 348
- lapse function, 245
- law
 - Einstein, 5
 - Newton, 5, 22, 138, 276
 - physical, 5
- Levi-Civita symbol, xix, 80, 327, 352, 409
- Lie algebra, 191, 502
 - Euclidean, 351, 354, 409
 - Poincaré, 409, 411
- Lie derivative, 495
- Lie group, 491, 492, 496, 504, 511
- light speed, 173
- Liouville theorem, 140
- local trivialization, 508
- Lorentz, 287
- Lorentz boost, 414

- Majorana equation, 207
- Majorana representation
 - alpha beta matrices, xix, 65
 - gamma matrices, xx, 65
- manifold, 286
 - differentiable, 286
- mass
 - electron, 145
- mass gap, 91, 107, 381, 386, 407
- mass parameter, 62
- massive, 415
- massless, 415
- mathematics
 - foundation of, 312
- matrix
 - Hamiltonian, 371, 377, 393
 - momentum, 362, 375, 410
 - wave operator, 357
- mean field, 104
- measure, 272
 - σ -finite, 465
 - Brownian Bridge, 277, 293, 483
 - centered, 472
 - characteristic functional, 343, 344, 465
 - correlation of, 72, 472
 - covariance of, 72, 472
 - degenerate, 473
 - equivalent, 467
 - finite, 6, 68
 - Gaussian, 277, 460
 - Lebesgue, 69, 292, 460
 - left invariant, 507
 - mean of, 472
 - mixed, 312, 479, 488
 - mutually singular, 467
 - product, 465
 - projector valued, 455
 - reverse Wiener, 304
 - right invariant, 507
 - spherical, 274
 - Stieltjes, 413
 - support, 490
 - support of, 296, 467, 483, 484
 - white noise, 291
 - Wiener, 280, 293, 483
- measure view, 328, 390, 403
- measurement, 74
 - direct, 139, 141, 144, 149, 433, 435
- mechanics, 5, 321, 429
 - statistical, 140, 429
- metric
 - background, 253
 - scaffold, 253
- metric tensor, 244
- mode, 237
 - coordinate, 237
- mode multi-index, 366
- molecule, 40
- momentum, 5, 84, 410
- monomial, 482
- monomial
 - anti-symmetric, 483
 - symmetric, 483
- multi-index, xix, xx, 30, 90, 226, 324, 360, 364
 - mode, 366
 - occupation, 366
- multiplicity, 336

- neutron, 221
- Newton, 6
- Newton gravitational constant, 244
- Newtonian motion path, 299
- nonrelativistic, 102
- normal evolution vector, 245
- normal mode, 95, 111
- normal subgroup, 501, 502
- normal vector, 245

- observable, 10, 25, 141, 321, 433
- occupation multi-index, 366, 419
- one-form, 494, 510
 - differential, 495
- open set, 492
- operator
 - annihilation, 95, 120, 361, 386
 - Casimir, 163, 414
 - confined wave, 90, 356
 - creation, 95, 120, 361, 386
 - cylinder, 360, 370
 - Fock, 49
 - Laplace, 347
 - mass-squared, 414
 - nabla, 338
 - Pauli-Lubanski, 414
 - quadratically confined wave, 356
 - resolvent, 44
 - self-adjoint, 25
 - statistical, 136, 445
 - unbounded, 74
 - wave, 91, 357
- operator-valued, 334
- orbit, 510
- orthochronous, 80, 501
- orthogonal transformation, 274, 349
- oscillator
 - harmonic, 229
 - harmonic, 29, 38, 47, 55, 89, 96, 196, 294, 479
 - quartic, 46, 112, 130
- paradox, 298
- parallel transport, 513
- particle-wave duality, 7, 22
- Pauli matrices, xix, 65, 170, 504
- pdf, 6, 140, 424
- permeability, 173
- permittivity, 173
- permutation symbol, xix
- perturbation theory, 42, 110, 112, 129
 - secular, 47
- photon, 223
- picture
 - Feynman, 55, 207
 - Heisenberg, 7, 13, 53, 74, 78, 142, 207, 208, 255, 334, 363
 - interaction, 76
 - Schrödinger, 7, 13, 53, 77, 142, 255, 323, 363, 380
 - Weyl, 204, 208, 231, 255
 - Wightman, 13, 79, 101, 118, 204, 205, 208, 231, 255, 334, 414
- piecewise definition, 367
- Plancherel formula, 342
- Planck length, 258
- pmf, 424
- Poincaré inequality, 454
- pointwise convergence, 404
- pointwise definition, 367
- Poisson bracket, 140, 432
- polylogarithm, 486
- polynomial, 84
 - anti-symmetric, 483
 - symmetric, 483
- positron, 193
- potential
 - polynomial, 66, 105, 368, 391, 394, 402, 416
 - quantum, 216
 - square well, 367
- probability, 22
 - density function, 140
 - distribution function, 6, 424
 - mass function, 424
- process
 - continuous, 425
 - deterministic, 427
 - discrete, 425
 - nondeterministic, 428
 - random, 425
 - stationary, 425
 - stochastic, 425
- product
 - Cartesian, 35, 139, 431, 460, 508
 - convolution, 214
 - semidirect, 79, 501, 502
 - tensor, 34, 35, 38, 40, 97, 102, 108, 118, 119, 127, 147, 203, 363, 402, 408, 413, 437–439, 460, 495
 - wedge, xx, 495
- projection map, 508
- propagator, 54, 214
- proton, 221
- pullback, 496
- pushforward, 495
- QCD, 223
- QED, 193
- quantum, 26, 417
- quantum chromodynamics, 223
- quantum electrodynamics, 193, 223
- quark, 221
- Radon-Nikodym derivative, 277, 379, 467, 477, 478
- random variable, 141, 424
 - basic, 426
 - dependent, 425
 - theoretical, 426
 - unobservable, 426
- rapidity, 311
- reality, 15
- realization, 331
- recurrence relation, 112
- renormalization, 162
 - conceptual, 163
- renormalization energy, 89, 90, 105, 107, 113, 114, 124, 163, 205, 228, 360, 370, 404–407
- representation, 414
 - adjoint, 176
 - decomposable, 86, 94, 97, 117, 287, 508
 - fundamental, 171, 172, 250
 - group, 287
 - irreducible, 86, 117, 287

542 Index

- reducible, 85, 287
- regular, 176
- reproducing kernel, 476
- Ricci tensor, 244
- Riemann-Christoffel tensor, 244

- sample value, 424
- scalar curvature, 244
- scalar product, 498
 - convention, xx
- scattering, 102, 127
 - matrix, 128
- SCF, 133
- Schmidt decomposition, 147
- section, 513
- secular terms, 46
- segment of sphere, 266
- self-adjoint, 276, 309
- self-consistent field, 48, 104, 133
- semisimple
 - Lie algebra, 503
 - Lie group, 503
- series
 - asymptotic, 45, 130
 - convergent, 45, 130
- sesquilinear, 499
- set
 - Borel, 340
 - convex, 271
 - cylinder, 72, 73, 299, 313, 344, 469, 470, 473, 476
- shift vector, 246
- SI units, 5, 39
- simple Lie algebra, 503
- simple Lie group, 503
- singular point
 - confluence, 112
 - irregular, 112
 - regular, 112
- Sommerfeld-Born formulation, 136
- space
 - Banach, 452
 - base, 189, 508
 - Cameron-Martin, 76, 77, 84, 87, 114, 211, 227, 274, 284, 296, 298, 345, 368, 474, 475, 477, 480–483
 - configuration, 4, 67, 201, 368
 - connected, 492
 - cotangent, 509
 - Euclidean, 513
 - fiber, 189, 508
 - Fock, xviii, 322, 363, 460
 - Hausdorff, 492
 - Hilbert, 7, 264, 331, 481
 - homogeneous, 511
 - principal, 511
 - horizontal, 513
 - linear, 264
 - measure, 344
 - metric, 265, 269, 451
 - Minkowski, 174
 - multiply connected, 493
 - of paths, 275
 - phase, 5, 6, 9, 23, 67, 137, 142, 201, 321, 429–431, 434
 - simply connected, 493
 - Sobolev, 276, 299, 332, 453, 483
 - symplectic, 28
 - tangent, 494, 509
 - topological, 492
 - total, 508
 - vertical, 513
- spacetime, xviii
- spectral gap, 91, 107, 381
- spectral representation, 43, 84, 131
- spectral representation function, 25, 67, 144, 151, 436
- spectral resolution, 455
- spectral sheet, 95, 115, 374, 408, 410
- spectral theorem, 347, 380, 455
- spectral transform, 11, 27, 38–40, 44, 52, 53, 63, 73, 84, 91, 93, 97, 101, 108, 115, 117, 125, 131, 132, 144, 147, 199, 203, 215, 229, 339, 340, 343, 346, 348, 349, 355, 368, 385, 386, 407, 408, 417, 419, 436
- spectrum, 117, 141
 - discrete, 455
- spinor, 64
 - adjoint, 198
 - Euler angles, 172, 198, 225
- srf, 25, 53, 67, 144, 436
- standard model, 221
- state, 5, 9, 10, 23
 - asymptotic, 102, 110
 - component, 439
 - dynamical, 23, 137, 141, 142, 151, 430, 431, 434
 - reduced, 439
 - statistical, 6, 14, 140, 141, 151, 431, 441
- statistical mechanics, 322
- statistical thermodynamics, 429
- Stieltjes integral, 306
- Stirling formula, 272
- structure constants, 176, 503
- submersion, 508
- sum
 - direct, 460
- superposition, 7, 10, 32
- supersymmetry, 202
- surface of sphere, 272
- symmetry, 286
 - gauge, 65
- symplectic, 143

- tempered distribution, 70
- tensor, 495
 - elementary, 438, 439
- theory
 - effective, 162, 219
 - measure, 6
 - quantum field, 6
 - relativity, 60, 286
 - Yang-Mills, 222, 223

- theory:constructive, 219
- thermodynamics
 - statistical, 140
- time slicing, 55, 290
- tip system, 444
- topological dual, xviii
- topology, 491
- trace class, 276, 324, 470, 472, 473, 481
- trace of operator, 281, 316, 317, 439, 470, 486
- trail marker, 1, 3, 9, 16, 19, 21, 28, 32, 39, 41,
 - 48, 50, 52, 55, 59, 62, 77, 86, 100,
 - 109, 121, 135, 152, 165, 167, 170,
 - 182, 193, 204, 209, 221, 224, 238,
 - 243, 261, 263, 264, 272, 289, 292,
 - 302, 314, 321, 351, 355, 367, 390,
 - 409, 418, 423, 442, 450
- ultralocal, 392
- uncertainty, 7, 15, 428, 431
- units, 173, 175
- vacuum, 85, 91, 114, 124, 131, 203, 212, 256,
 - 368
- variable
 - classical, 15
 - dynamical, 12, 67, 138, 142, 149, 154, 183,
 - 184, 189, 196, 197, 206, 207, 228,
 - 247, 431, 435, 444
 - macroscopic, 14, 15, 156, 443, 447
- version
 - gauge field solution, 187
 - measurable function, 332, 337, 378, 481, 482
- virtual particle, 101
- visualization
 - of Hilbert space, 270
 - of interior and surface, 273, 284
 - of path spaces, 283
- volume of ball, 272
- wave function, 7, 15, 24, 142, 436
 - collapse, 15, 162
- wave functional, 68
- wedge
 - of sphere, 267
 - root of, 267
 - tip of, 267
- Yang-Mills field strength, 176
- Yang-Mills potential, 176