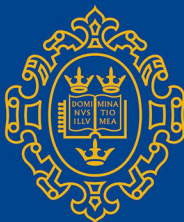


Quantum Statistical Field Theory

An Introduction to Schwinger's Variational
Method with Green's Function Nanoapplications,
Graphene and Superconductivity

NORMAN J. MORGENSTERN HORING



OXFORD SCIENCE PUBLICATIONS

INTERNATIONAL SERIES OF MONOGRAPHS ON PHYSICS

SERIES EDITORS

J. BIRMAN	City University of New York
S. F. EDWARDS	University of Cambridge
R. FRIEND	University of Cambridge
M. REES	University of Cambridge
D. SHERRINGTON	University of Oxford
G. VENEZIANO	CERN, Geneva

INTERNATIONAL SERIES OF MONOGRAPHS ON PHYSICS

166. N. Horing: *Quantum statistical field theory*
165. T.C. Choy: *Effective medium theory, Second edition*
164. L. Pitaevskii, S. Stringari: *Bose-Einstein condensation and superfluidity*
163. B.J. Dalton, J. Jeffers, S.M. Barnett: *Phase space methods for degenerate quantum gases*
162. W.D. McComb: *Homogeneous, isotropic turbulence - phenomenology, renormalization and statistical closures*
161. V.Z. Kresin, H. Morawitz, S.A. Wolf: *Superconducting state - mechanisms and properties*
160. C. Barrabès, P.A. Hogan: *Advanced general relativity - gravity waves, spinning particles, and black holes*
159. W. Barford: *Electronic and optical properties of conjugated polymers, Second edition*
158. F. Strocchi: *An introduction to non-perturbative foundations of quantum field theory*
157. K.H. Bennemann, J.B. Ketterson: *Novel superfluids, Volume 2*
156. K.H. Bennemann, J.B. Ketterson: *Novel superfluids, Volume 1*
155. C. Kiefer: *Quantum gravity, Third edition*
154. L. Mestel: *Stellar magnetism, Second edition*
153. R.A. Klemm: *Layered superconductors, Volume 1*
152. E.L. Wolf: *Principles of electron tunneling spectroscopy, Second edition*
151. R. Blinc: *Advanced ferroelectricity*
150. L. Berthier, G. Biroli, J.-P. Bouchaud, W. van Saarloos, L. Cipelletti: *Dynamical heterogeneities in glasses, colloids, and granular media*
149. J. Wesson: *Tokamaks, Fourth edition*
148. H. Asada, T. Futamase, P. Hogan: *Equations of motion in general relativity*
147. A. Yaouanc, P. Dalmas de Réotier: *Muon spin rotation, relaxation, and resonance*
146. B. McCoy: *Advanced statistical mechanics*
145. M. Bordag, G.L. Klimchitskaya, U. Mohideen, V.M. Mostepanenko: *Advances in the Casimir effect*
144. T.R. Field: *Electromagnetic scattering from random media*
143. W. Götz: *Complex dynamics of glass-forming liquids - a mode-coupling theory*
142. V.M. Agranovich: *Excitations in organic solids*
141. W.T. Grandy: *Entropy and the time evolution of macroscopic systems*
140. M. Alcubierre: *Introduction to 3+1 numerical relativity*
139. A.L. Ivanov, S.G. Tikhodeev: *Problems of condensed matter physics - quantum coherence phenomena in electron-hole and coupled matter-light systems*
138. I.M. Vardavas, F.W. Taylor: *Radiation and climate*
137. A.F. Borghesani: *Ions and electrons in liquid helium*
135. V. Fortov, I. Iakubov, A. Khrapak: *Physics of strongly coupled plasma*
134. G. Fredrickson: *The equilibrium theory of inhomogeneous polymers*
133. H. Suhl: *Relaxation processes in micromagnetics*
132. J. Terning: *Modern supersymmetry*
131. M. Mariño: *Chern-Simons theory, matrix models, and topological strings*
130. V. Gantmakher: *Electrons and disorder in solids*
129. W. Barford: *Electronic and optical properties of conjugated polymers*
128. R.E. Raab, O.L. de Lange: *Multipole theory in electromagnetism*
127. A. Larkin, A. Varlamov: *Theory of fluctuations in superconductors*
126. P. Goldbart, N. Goldenfeld, D. Sherrington: *Stealing the gold*
125. S. Atzeni, J. Meyer-ter-Vehn: *The physics of inertial fusion*
123. T. Fujimoto: *Plasma spectroscopy*
122. K. Fujikawa, H. Suzuki: *Path integrals and quantum anomalies*
121. T. Giamarchi: *Quantum physics in one dimension*
120. M. Warner, E. Terentjev: *Liquid crystal elastomers*
119. L. Jacak, P. Sitko, K. Wieczorek, A. Wojs: *Quantum hall systems*
117. G. Volovik: *The Universe in a helium droplet*
116. L. Pitaevskii, S. Stringari: *Bose-Einstein condensation*
115. G. Dissertori, I.G. Knowles, M. Schmelling: *Quantum chromodynamics*
114. B. DeWitt: *The global approach to quantum field theory*
113. J. Zinn-Justin: *Quantum field theory and critical phenomena, Fourth edition*
112. R.M. Mazo: *Brownian motion - fluctuations, dynamics, and applications*
111. H. Nishimori: *Statistical physics of spin glasses and information processing - an introduction*
110. N.B. Kopnin: *Theory of nonequilibrium superconductivity*
109. A. Aharoni: *Introduction to the theory of ferromagnetism, Second edition*
108. R. Dobbbs: *Helium three*
107. R. Wigmans: *Calorimetry*
106. J. Kübler: *Theory of itinerant electron magnetism*
105. Y. Kuramoto, Y. Kitaoka: *Dynamics of heavy electrons*
104. D. Bardin, G. Passarino: *The Standard Model in the making*
103. G.C. Branco, L. Lavoura, J.P. Silva: *CP Violation*
101. H. Araki: *Mathematical theory of quantum fields*
100. L.M. Pismen: *Vortices in nonlinear fields*

Quantum Statistical Field Theory

An Introduction to Schwinger's Variational Method
with Green's Function Nanoapplications, Graphene
and Superconductivity

Norman J. Morgenstern Horing

Department of Physics and Engineering Physics, Stevens Institute of Technology

OXFORD
UNIVERSITY PRESS

OXFORD
UNIVERSITY PRESS

Great Clarendon Street, Oxford, OX2 6DP,
United Kingdom

Oxford University Press is a department of the University of Oxford.
It furthers the University's objective of excellence in research, scholarship,
and education by publishing worldwide. Oxford is a registered trade mark of
Oxford University Press in the UK and in certain other countries

© Norman J. Morgenstern Horing 2017

The moral rights of the author have been asserted

First Edition published in 2017

Impression: 1

All rights reserved. No part of this publication may be reproduced, stored in
a retrieval system, or transmitted, in any form or by any means, without the
prior permission in writing of Oxford University Press, or as expressly permitted
by law, by licence or under terms agreed with the appropriate reprographics
rights organization. Enquiries concerning reproduction outside the scope of the
above should be sent to the Rights Department, Oxford University Press, at the
address above

You must not circulate this work in any other form
and you must impose this same condition on any acquirer

Published in the United States of America by Oxford University Press
198 Madison Avenue, New York, NY 10016, United States of America

British Library Cataloguing in Publication Data
Data available

Library of Congress Control Number: 2016952831

ISBN 978-0-19-879194-2

Printed in Great Britain by
CPI Group (UK) Ltd, Croydon, CR0 4YY

Links to third party websites are provided by Oxford in good faith and
for information only. Oxford disclaims any responsibility for the materials
contained in any third party website referenced in this work.

Rose Morgenstern Horing

1911–1999

*Deeply loved mother and protector who, in the worst of times, braved severe adversity
and privation to deliver me to manhood*

Norman J. Morgenstern Horing

Contents

Prologue	xiii
Acknowledgments	xvii
1 Dirac Notation and Transformation Theory	1
1.1 Introductory Review	1
1.2 Dirac Notation	8
1.3 Complete Sets of Commuting Observables, Representations and Transformation Theory	13
1.4 Schwinger Measurement Symbols	15
1.5 Chapter 1 Problems	16
1.6 References for Chapter 1	19
2 Identical Particles and Second Quantization: Occupation Number Representation	20
2.1 Operators for Properties of Identical Particles	20
2.2 Second Quantization: Occupation Number Representation	24
2.3 Coherent States, Squeezed States	33
2.4 Chapter 2 Problems	38
2.5 References for Chapter 2	39
3 Q. M. Pictures; Heisenberg Equation; Linear Response; Superoperators and Non-Markovian Equations	40
3.1 Schrödinger Picture: Iteration Series for the Time-Development Operator	41
3.2 Heisenberg Picture and Equations of Motion	44
3.3 Interaction Picture	47
3.4 Linear Response	51
3.5 S-Matrix, Density Matrix, Superoperators and Non-Markovian Kinetic Equations	53
3.6 Chapter 3 Problems	59
3.7 References for Chapter 3	60
4 Schwinger Action Principle and Variational Calculus	61
4.1 Action Principle: Quantum Hamilton Equations	61
4.2 Variational Calculus and Sources	72
4.3 Particle Sources: General Considerations	81
4.4 Potential Source: General Considerations	87

4.5	An Identity	91
4.6	Chapter 4 Problems	93
4.7	References for Chapter 4	93
5	Retarded Green's Functions	95
5.1	Definition, Equation of Motion and Interpretation of Retarded Green's Functions	95
5.2	Partial Green's Functions, Applications to Localized States in a Continuum and Chemisorption	101
5.3	Dyson Integral Equation, T-Matrix for $\delta(\mathbf{x})$ -Function Potential	105
5.4	Random Impurity Scattering: Born and Self-Consistent Born Approximations	107
5.5	Ando's Semi-Elliptic Density of States for the 2D Landau-Quantized Electron-Impurity System	113
5.6	Magnetic Field Green's Function for Electrons in Three and Two Dimensions	116
5.7	Green's Function Determination by Hamilton Equations: 2D Saddle Potential in $\mathbf{E}(t)$ Field	123
5.8	Product Green's Functions for Separable Hamiltonians: 1D Superlattice in Axial Fields	127
5.9	Electron Propagation in a Heterostructure with Spatially Variable Mass: Green's Function Matching	133
5.10	Green's Function Matching: Dynamic, Non-Local Electrostatic Screening at Interface; Surface Plasmons	138
5.11	Feynman Path Integrals	144
5.12	Chapter 5 Problems	145
5.13	References for Chapter 5	148
6	Quantum Mechanical Ensemble Averages and Statistical Thermodynamics	150
6.1	Quantum Mechanical Ensemble Averages and Thermodynamics	150
6.2	Boson and Fermion Statistics for Non-Interacting Systems: Bose Condensation	156
6.3	Helmholtz Free Energy and Magnetic Moment	159
6.4	Diamagnetic Susceptibility and the de Haas-van Alphen Effect	163
6.5	Chapter 6 Problems	166
6.6	References for Chapter 6	167
7	Thermodynamic Green's Functions and Spectral Structure	168
7.1	Definition and Interpretation of Thermal Green's Functions	168
7.2	Lehmann Spectral Representation of the One-Particle Thermal Green's Function	169
7.3	Other Spectral Considerations	173
7.4	Periodicity/Antiperiodicity in Imaginary Time, Matsubara Frequencies and Analytic Continuation	174

7.5	Commutator/Anticommutator Functions; Retarded/Advanced Green's Functions; Spectral Sum Rule	179
7.6	Statistical Thermodynamic Information in the One- and Two-Particle Green's Functions	182
7.7	Chapter 7 Problems	185
7.8	References for Chapter 7	186
8	Equations of Motion with Particle-Particle Interactions and Approximations	187
8.1	Multiparticle Green's Function Equations of Motion	188
8.2	Non-Correlation Decoupling Procedures for G_2 : Hartree and Hartree-Fock Approximations	191
8.3	Non-Correlation Decoupling Procedures: Collisional Effects; <i>Sum of Ladder Diagrams</i> Integral Equation	195
8.4	Electron-Hole Interaction: Exciton States	198
8.5	Chapter 8 Problems	204
8.6	References for Chapter 8	205
9	Non-Equilibrium Green's Functions: Variational Relations and Approximations for Particle Interactions	206
9.1	Non-Equilibrium Green's Functions, Definitions and Variational Relations in Terms of Particle Sources	207
9.2	Exact Variational Relations in Terms of a Source Potential	216
9.3	Cumulants and the Linked Cluster Theorem	218
9.4	Variational Differential Formulation of the Random Phase Approximation	221
9.5	Variational Differential Formulation of Perturbation Theory	225
9.6	Self-Energy and Vertex Operator Perturbation Theory	227
9.7	Shielded Potential Perturbation Theory	229
9.8	Imaginary Time, Contour Time Ordering and the Langreth Algebra	231
9.9	Generalized Kadanoff-Baym Ansatz for Derivation of Quantum Transport Equations	234
9.10	Chapter 9 Problems	236
9.11	References for Chapter 9	237
10	Random Phase Approximation Plasma Phenomenology, Semiclassical and Hydrodynamic Models; Electrodynamics	238
10.1	Dielectric Response Functions for Inhomogeneous and Homogeneous Systems	239
10.2	RPA Plasmons and Shielding in 3D, 2D and 1D, Magnetoplasmas, Models and Surface Plasmons	244
10.3	Exchange and Correlation Energy	252

10.4	Atom–Surface van der Waals Attraction; Physisorption and the Plasma Image	256
10.5	Fast Particle Power Loss in Plasma	264
10.6	Electrodynamic Dielectric Response Functions for Quantum Plasmas: Dyadic Green’s Functions	271
10.7	Dynamic, Non-Local Conductivity and Inverse Dielectric Tensors	280
10.8	Polaritons in Compound Nanostructures	290
10.9	Chapter 10 Problems	299
10.10	References for Chapter 10	300
11	Interacting Electron–Hole–Phonon System	302
11.1	Electron–Hole–Phonon Interaction Hamiltonian	303
11.2	Coupled Electron–Hole–Phonon Green’s Functions and Equations	307
11.3	Electron–Phonon Interaction Phenomenology	314
11.4	Alternative Formulation of the Equations of Motion	323
11.5	Analysis of Electron–Hole Interaction Dynamics	327
11.6	Generalized Shielded Potential Approximation: Electron–Hole Interaction Operator	330
11.7	Dielectric Response of the Electron–Hole–Phonon System	333
11.8	Exciton–Plasmon Interaction	337
11.9	Chapter 11 Problems	338
11.10	References for Chapter 11	338
12	Graphene	340
12.1	Introduction	340
12.2	Graphene Hamiltonian, Green’s Function and Dielectric Function	341
12.3	Graphene Green’s Function in a Perpendicular Magnetic Field: Landau Quantization	346
12.4	Graphene Quantum Dot: Magnetic Field Green’s Function	352
12.5	Graphene Antidot Lattice in a Magnetic Field	355
12.6	Graphene Statistical Thermodynamics and Magnetic Moment	358
12.7	Further Remarks and Developments	361
12.8	Chapter 12 Problems	363
12.9	References for Chapter 12	364
13	Superfluidity and Superconductivity	370
13.1	Superfluid Field Operators and the Gross–Pitaevskii Equations	371
13.2	Superfluid Green’s Functions and Elementary Excitations	375

13.3	Superconductivity: BCS Theory; Anomalous Green's Functions and Gorkov Equations	382
13.4	Excitation Spectrum, Gap; Isotope Effect	386
13.5	Thermodynamics of Superconductors	389
13.6	Ginzburg–Landau Theory	391
13.7	London Theory; Meissner Effect	397
13.8	Electromagnetic Current Response of Superconductors: Gauge Invariance and Collective Modes	399
13.9	Magnetic Flux Quantization: Type I and Type II Superconductors	408
13.10	Josephson Tunneling	412
13.11	Further Remarks and Developments	415
13.12	Chapter 13 Problems	418
13.13	References for Chapter 13	418
Epilogue		421
Index		429

Prologue

Since the landmark breakthroughs in quantum electrodynamics, *c.*1950, the methods of advanced quantum mechanics, in particular Green's functions, have been the preferred and principal tools for theoretical research on the fundamental physics of particles and matter. Their use has facilitated the systematization of highly complicated analyses in the relativistic theory of interacting quantum fields, leading to profoundly important (indeed, Nobel prize-winning) developments, in the context of both variational differential methods and equivalent Feynman-diagrammatic methods. The transfer of these methods into the non-relativistic domain of condensed matter theory has also led to immensely improved understanding of the electronic properties of metals, semiconductors, superconductors, superfluids, magnetism, etc. Again, the use of Green's functions by physicists led to extraordinary scientific advances, not only in regard to the prediction and explanation of physical phenomena, but also in providing insight into the development of new devices. With this, physics is once again spawning new engineering disciplines, as it has done in the past with electronic, optical and nuclear engineering. It is now fairly common to find electrical engineering (as well as applied physics) departments around the world heavily staffed with faculty deeply involved in research in areas such as charge transport in semiconductors, nanostructures, quantum tunneling, superconductivity, etc.: areas of research that are well served by the use of Green's functions, to which engineering researchers increasingly turn to penetrate difficult problems.

This book has grown out of a two-semester course on the methods of advanced quantum mechanics that I have taught at Stevens Institute of Technology over many years. It is mainly based on the lectures of Professor Julian Schwinger at Harvard University (*c.*1956) and the seminal paper of P. C. Martin and J. Schwinger, followed by important contributions of their students and others. The book is eclectic in the material addressed from many points of view. It makes no reference to Feynman diagrammatics, as that subject already permeates the literature, but it does introduce superoperators; quantum-mechanical Green's functions are discussed in detail, but their applications are selectively limited while classical electromagnetic dyadic Green's functions are treated in this book on quantum theoretical methods; moreover, Landau diamagnetism is included, but ferromagnetism is not. In reality, a much fuller book of this type could and should have been written by Schwinger and/or Martin, but, unfortunately, that has not happened, although some of Schwinger's notes at the University of California at Los Angeles were published in his name in "Quantum Mechanics," edited by B. G. Englert, Springer (2001). If that book had gone further, it would have totally eclipsed this one. However, it did leave a bit of room for additional presentations (with some overlap).

This book has two objectives. The first is pedagogical, addressing students of science and engineering who have had just a first exposure to quantum mechanics in terms of the

one-particle Schrödinger equation on the level of A. Beiser's book "Concepts of Modern Physics" or R. L. Liboff's "Introductory Quantum Mechanics." The present book is intended to introduce them to the advanced aspects of quantum mechanics that are important in current, mainly non-relativistic, research on interacting quantum systems. These include correlation phenomena due to electron–electron interactions, collective modes, electron–hole interactions, electron–phonon interactions, Graphene, superfluids, superconductors, magnetism, and semiconductor nanostructures that play a central role in the high-tech thrust for smaller, faster devices to facilitate the development of more powerful computers and other electronic devices. There are several mechanisms that I feel will help to rapidly advance the educational status of students of modest background in the arena of condensed matter quantum physics and engineering, to bring the reader to the point of being able to understand modern theoretical research papers and carry out such research themselves. One such mechanism is Schwinger's interpretation of Dirac ket-bra dyads in terms of *measurement symbols* that are factorized into annihilation and creation operators to introduce second quantization, which I consider to be more efficient educationally than other approaches to the subject. (Its effectiveness is undiminished by Schwinger's later adoption of a somewhat different notation.) Another mechanism is the use of variational differentiation jointly with the Schwinger Action Principle to mathematically describe interacting quantum systems and formulate various perturbation theories for them at arbitrary temperature and under non-equilibrium conditions, without explicit recourse to Wick's theorem. Providing the bit of introduction to variational calculus (in Chapter 4) that the reader needs is a small price to pay for the much greater efficiency of variational differential techniques. Such improved educational mechanisms have proved beneficial to rapidly advancing students' capabilities in the past. For example, the introduction of Dirac notation has certainly facilitated the study of quantum mechanics and the Dirac delta-function is employed universally because of its great utility. Vector calculus with its grad, div, curl makes it much easier to learn (as well as teach) potential theory and electromagnetics. Venerable older books like Kellogg's "Potential Theory" and Sir James Jeans' "The Mathematical Theory of Electricity and Magnetism" present derivations that seem painfully lengthy in comparison with more modern and efficient presentations. Variational techniques offer such efficiencies of presentation, which we employ here for the reader's benefit. In some instances our explication/derivation of the material is detailed to the point of exhausting the patience of more knowledgeable readers, but it has been effective in promoting understanding of the subject in lower level students, including some mathematically strong undergraduates. While the material has traditionally been viewed as "advanced," the primary object here is to present it on an intermediate level using Schwinger's variational methods.

The second purpose of this book is to provide the reader with examples of applications to recent research on semiconductor nanostructures, including low-dimensional systems and Graphene. Introductions to the microscopic theories of superfluids and superconductors are included, as well as various facets of magnetic Landau quantization of electron orbits.

Following introductory chapters on Dirac notation, second quantization (including coherent states), Schrödinger, Heisenberg and Interaction Pictures and superoperators,

Chapter 4 presents the Schwinger Action Principle (encompassing all aspects of quantum theory) and variational calculus. An introduction to retarded Green's functions, the Dyson equation and T -matrix for a $\delta(\mathbf{x})$ -potential, as well as for random impurity scattering, is presented in Chapter 5, where the self-consistent Born approximation is discussed. Partial Green's functions are also treated, with application to chemisorption, and the technique of Green's function matching is derived and applied to the Schrödinger equation and surface plasmons. Chapter 6 reviews some of the essentials of quantum statistical mechanics, ensemble theory and statistical thermodynamics, including the de Haas–van Alphen effect.

Thermal Green's functions and their spectral structure are presented in detail in Chapter 7, including the Lehmann spectral representation, periodicity/antiperiodicity in imaginary time, Matsubara frequencies, analytic continuation and the spectral sum rule. The equations of motion for multiparticle Green's functions with particle–particle interactions and non-correlation decoupling procedures, including the Ladder Diagram integral equation, are derived in Chapter 8, with application to electron–hole exciton states. Non-equilibrium Green's functions are introduced in Chapter 9 and exact variational relations in terms of particle and potential sources are presented. Cumulants and the Linked Cluster Theorem are discussed, as is a variational differential formulation of the random phase approximation (RPA). Variational differential formulations of perturbation theories for Green's functions, self-energy and vertex operators, as well as the shielded potential approximation, are derived, and the Langreth Algebra is discussed as well as the Generalized Kadanoff–Baym Ansatz. Chapter 10 is concerned with RPA plasma phenomenology and models, including dynamic, non-local dielectric response, plasmons, shielding, exchange and correlation energy, with an application to atom–surface van der Waals physisorption. Electromagnetic dyadic Green's functions are also discussed in Chapter 10, along with dynamic, non-local conductivity and dielectric tensors with applications to polaritons in compound nanostructures. A model of the interacting electron–hole–phonon system is treated in detail in Chapter 11, with an introductory discussion of the model Hamiltonian and definition and derivation of equations of motion for the coupled Green's functions of the system. An alternative formulation of the equations of motion with *five* interactions (electron–electron, hole–hole, electron–hole, electron–phonon and hole–phonon) is presented to facilitate the development of a generalized shielded potential approximation for this extremely complex system: A representation of the dynamics of such a system having five interactions would present a serious challenge to a Feynman-diagrammatic formulation. The subject of Graphene is introduced and discussed in Chapter 12. Finally, an extended introduction to the microscopic theories of superfluids and superconductors is presented in Chapter 13 and an Epilogue indicating directions for further reading is provided.

Acknowledgments

In appreciation of the fine education provided by Professors Mark Zemansky, Larry Wills, Roy Glauber, Paul Martin and Julian Schwinger, and the other denizens of the deep at the City College of New York (CUNY) and Harvard University.

With eternal appreciation for the steadfast support, encouragement,

and love of my wife

Jerilyn

in this long and difficult journey.

N.J.M.H.

Dirac Notation and Transformation Theory

Abstract

Chapter 1 opens with a brief review of some basic features of quantum mechanics, including the Schrödinger equation, linear and angular momentum and the theory of the hydrogenic atom. It also includes complete orthonormal sets of eigenfunctions, the translation operator, current, spin, equation of continuity, gauge transformation, determinant and permanent multiparticle energy eigenfunctions and the Pauli exclusion principle. Attention is then focused on Dirac bra-ket notation and complete sets of commuting observables. In this connection, representations and transformation among representations are discussed in detail for the Schrödinger system state vector and the eigenstates, as well as bra-ket matrix elements of operators. Finally, Schwinger's interpretation of ket-bra matrix operator structures in terms of annihilation and creation of systems in eigenstates is introduced.

1.1 Introductory Review

In a first exposure to quantum mechanics, the Hamiltonian, $H(\mathbf{x}, \mathbf{p})$, for a single particle is usually written in position representation as $H(\mathbf{x}, \frac{\hbar}{i}\nabla)$ and the quantum dynamical time development of the wave function $\Psi(\mathbf{x}, t)$ is determined by the single-particle Schrödinger equation,¹⁻³

$$H(\mathbf{x}, \frac{\hbar}{i}\nabla)\Psi(\mathbf{x}, t) = i\hbar \frac{\partial \Psi(\mathbf{x}, t)}{\partial t}, \quad (1.1.1)$$

where $\mathbf{p} = \frac{\hbar}{i}\nabla$ is the momentum operator in position representation. The probability density for the particle to be found at $\mathbf{x}$ at time t is $|\Psi(\mathbf{x}, t)|^2$. Solutions for $\Psi(\mathbf{x}, t)$ are often sought by expansion in the complete orthonormal set of eigenfunctions $\phi_r(\mathbf{x})$ associated with a Hermitian operator $\Theta(\mathbf{x}, \frac{\hbar}{i}\nabla)$ having eigenvalues λ_r :

$$\Theta(\mathbf{x}, \frac{\hbar}{i}\nabla)\phi_r(\mathbf{x}) = \lambda_r\phi_r(\mathbf{x}), \quad (1.1.2)$$

and Θ is frequently (but not necessarily) chosen as a part of H that is relatively easy to analyze. The completeness and orthonormality of the eigenfunctions $\phi_r(\mathbf{x})$ may be expressed as follows ($\delta_{rs} = 1, 0$ for $r = s, r \neq s$ is the Kronecker delta):

$$\text{Completeness: } \Psi(\mathbf{x}, t) = \sum_r C_r(t) \phi_r(\mathbf{x}), \quad (1.1.3)$$

$$\text{Orthonormality: } \int d^{(3)}\mathbf{x} \phi_r^*(\mathbf{x}) \phi_s(\mathbf{x}) = \delta_{rs}, \quad (1.1.4)$$

which lead to C_r expressed as

$$C_r(t) = \int d^{(3)}\mathbf{x} \phi_r^*(\mathbf{x}) \Psi(\mathbf{x}, t). \quad (1.1.5)$$

An alternative expression of completeness is given by

$$\sum_r \phi_r^*(\mathbf{x}') \phi_r(\mathbf{x}) = \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (1.1.6)$$

where $\delta^{(3)}(\mathbf{x} - \mathbf{x}')$ is a three-dimensional (3D) Dirac delta function,^{4,5} which plays the same role under integration as does the Kronecker delta, δ_{ij} , under summation.

A simple, but important, example is provided by choosing Θ to be the momentum operator, $\Theta = \mathbf{p} \Rightarrow \frac{\hbar}{i} \nabla$. Its components, p_j , obey canonical commutation relations with coordinate components, $x_i : [x_i, p_j] \equiv (x_i p_j - p_j x_i) = i\hbar \delta_{ij}$. The eigenfunction equation, $\frac{\hbar}{i} \nabla \phi(\mathbf{x}) = \lambda \phi(\mathbf{x})$, has a continuum of infinite space eigenvalues, $\lambda \rightarrow \mathbf{p}'$ (all real 3-vector momenta), with the corresponding eigenfunctions $\phi_{\mathbf{p}'}(\mathbf{x}) = \exp(i \frac{\mathbf{p}'}{\hbar} \cdot \mathbf{x}) / (2\pi\hbar)^{3/2}$. The completeness relation, Eq. (1.1.3), is then just the Fourier transform, $\Psi(\mathbf{x}, t) = \int \frac{d^{(3)}\mathbf{p}'}{(2\pi\hbar)^{3/2}} \exp(i \frac{\mathbf{p}'}{\hbar} \cdot \mathbf{x}) C_{\mathbf{p}'}(t)$, which leads to Eq. (1.1.6) in the form $\int \frac{d^{(3)}\mathbf{p}'}{(2\pi\hbar)^3} \exp(i \frac{\mathbf{p}'}{\hbar} \cdot \mathbf{x}) \exp(-i \frac{\mathbf{p}'}{\hbar} \cdot \mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}')$ as a known identity, and the continuum form of the orthonormality relation, Eq. (1.1.4), is given by $\int \frac{d^{(3)}\mathbf{x}}{(2\pi\hbar)^3} \exp(i \frac{\mathbf{p}'}{\hbar} \cdot \mathbf{x}) \exp(-i \frac{\mathbf{p}''}{\hbar} \cdot \mathbf{x}) = \delta^{(3)}(\mathbf{p}' - \mathbf{p}'')$. It is important to note that the momentum operator, $\mathbf{p} = \frac{\hbar}{i} \nabla$, generates spatial translations since the 3D Taylor series for a positional displacement of $f(\mathbf{x})$ through $\mathbf{a}$ may be written as

$$f(\mathbf{x} + \mathbf{a}) = \sum_{n=0}^{\infty} \frac{(\mathbf{a} \cdot \nabla)^n}{n!} f(\mathbf{x}) = \exp(\mathbf{a} \cdot \nabla) f(\mathbf{x}) = \exp\left(\frac{i}{\hbar} \mathbf{a} \cdot \mathbf{p}\right) f(\mathbf{x}). \quad (1.1.7)$$

There are some systems of great intrinsic physical interest with correspondingly important Hamiltonians that can be treated exactly. In this regard, we briefly review the properties of H for a Coulombic force center, which is of special interest in connection with the theory of excitons to be discussed in a later chapter. The hydrogenic atom, which was of central significance in the historical development of quantum theory, involves the well-known Hamiltonian (Z is the charge number of the nucleus and r is the radial distance from it):

$$H = \frac{-\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{r} = \frac{-\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\mathbf{L}^2}{2mr^2} - \frac{Ze^2}{r}. \quad (1.1.8)$$

The last term represents the Coulomb potential attracting the electron to the nuclear center. Here, $\mathbf{L}$ is the quantum mechanical orbital angular momentum operator for a single particle, defined by

$$\mathbf{L} = \mathbf{x} \times \mathbf{p} = \mathbf{x} \times \frac{\hbar}{i} \nabla. \quad (1.1.9)$$

Its Cartesian components, L_i ($i = 1, 2, 3$), obey the commutation relations

$$[L_i, L_j] = i\hbar \sum_{k=1}^3 \varepsilon_{ijk} L_k, \quad (1.1.10)$$

where ε_{ijk} is 1, -1 if i, j, k is an even, odd permutation of 1, 2, 3 and it vanishes if any index is repeated. In spherical coordinates (θ is polar angle, ϕ is azimuthal angle), we have

$$\begin{aligned} L_1 &= \frac{\hbar}{i} \left(-\sin \phi \frac{\partial}{\partial \theta} - \cos \phi \cot \theta \frac{\partial}{\partial \phi} \right), \\ L_2 &= \frac{\hbar}{i} \left(\cos \phi \frac{\partial}{\partial \theta} - \sin \phi \cot \theta \frac{\partial}{\partial \phi} \right), \\ L_3 &= \frac{\hbar}{i} \frac{\partial}{\partial \phi}, \end{aligned} \quad (1.1.11)$$

and

$$\mathbf{L}^2 = \sum_{i=1}^3 L_i^2 = -\hbar^2 \left[\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \right]. \quad (1.1.12)$$

Just as the momentum operator generates spatial translations, it is readily seen from Eq. (1.1.11) that L_3 generates spatial rotations about the 3-axis. The eigenfunctions and eigenvalue spectrum of $\mathbf{L}^2$ are given by

$$\mathbf{L}^2 \varphi_{l,m} = \hbar^2 l(l+1) \varphi_{l,m}, \text{ where the orbital quantum number is } l = 0, 1, 2 \dots \infty, \quad (1.1.13)$$

$\varphi_{l,m} = Y_l^m(\theta, \phi)$ is a spherical harmonic with

$$L_3 \varphi_{l,m} = \hbar m \varphi_{l,m} \text{ and the magnetic quantum number is } m = -l \dots 0 \dots +l. \quad (1.1.14)$$

The separable energy eigenfunctions of H for a hydrogenic atom having the Hamiltonian of Eq. (1.1.8),

$$H \Phi_{n,l,m} = E_{n,l,m} \Phi_{n,l,m}, \quad (1.1.15)$$

which are simultaneously eigenfunctions of $\mathbf{L}^2$ and L_3 (Eqns. (1.1.13 and 1.1.14)) are given by (we define $R_n = 2Zr/a_0n$, where a_0 is the Bohr radius):

$$\Phi_{n,l,m}(r, \theta, \phi) = \left(\frac{2Z}{a_0 n} \right)^{\frac{3}{2}} A_{nl}(R_n)^l e^{-\frac{R_n}{2}} F_{nl}(R_n) Y_l^m(\theta, \phi), \quad (1.1.16)$$

with energy eigenvalues

$$E_{n,l,m} = E_n = \frac{-Z^2 e^2}{2a_0 n^2} \quad (1.1.17)$$

(degenerate in l, m), where the principal quantum number n is an integer $n > l$, $F_{nl}(R_n)$ is an associated Laguerre polynomial, and normalization to unity is provided by

$$A_{nl} = \sqrt{\frac{(n-l-1)!}{2n[(n+l)!]^3}}. \quad (1.1.18)$$

The spatial localization of these energy eigenfunctions associated with the discrete character of the spectrum is evident from the factor $e^{-R_n/2}$.

The classical relation between the orbital angular momentum $\mathbf{L}$ of a particle of charge Q , mass m and its magnetic moment $\boldsymbol{\mu}$ also holds for the associated quantum mechanical operators,

$$\boldsymbol{\mu} = \frac{Q}{2mc} \mathbf{L}. \quad (1.1.19)$$

(Of course, there are anomalies due to interactions.) The analysis of atomic spectra made it clear that there is yet another internal coordinate related to an intrinsic magnetic moment of the electron and its associated intrinsic angular momentum, $\mathbf{S}$, which could take just two values, $S_z \rightarrow \pm \frac{\hbar}{2}$. As angular momenta (intrinsic as well as orbital), these operators obey the characteristic commutation relations, Eq. (1.1.10),

$$[S_i, S_j] = i\hbar \sum_{k=1}^3 \varepsilon_{ijk} S_k. \quad (1.1.20)$$

Since they can only have two eigenvalues, they may be described by 2×2 Pauli spin matrices,

$$\boldsymbol{\sigma} = \frac{2}{\hbar} \mathbf{S}, \quad (1.1.21)$$

which obey similar relations:

$$[\sigma_i, \sigma_j] = 2i \sum_{k=1}^3 \varepsilon_{ijk} \sigma_k. \quad (1.1.22)$$

A convenient representation is given by $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$; $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$; $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The Pauli matrices are Hermitian, idempotent and *anticommutative* in accordance with the relations (I is the unit 2×2 matrix, $i, j = 1, 2, 3$):

$$\sigma_i \sigma_j = I \delta_{ij} + i \sum_{k=1}^3 \varepsilon_{ijk} \sigma_k \quad (1.1.23)$$

and

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2I \delta_{ij}. \quad (1.1.24)$$

The associated intrinsic magnetic moment of the electron is given by

$$\boldsymbol{\mu}_s = \frac{-e}{mc} \mathbf{S} \quad \text{corresponding to} \quad \mu_{sz} \implies \pm \frac{e\hbar}{2mc}, \quad (1.1.25)$$

since the gyromagnetic ratio for electron spin is approximately twice that of the orbital angular momentum. The total angular momentum operator for an electron is given by

$$\vec{\mathcal{J}} = \mathbf{L} + \mathbf{S}. \quad (1.1.26)$$

In the presence of an electromagnetic field having vector and scalar potentials, $\mathbf{A}(\mathbf{x}, t)$ and $\phi(\mathbf{x}, t)$, respectively, with $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\nabla\phi - \frac{1}{c}\partial\mathbf{A}/\partial t$, the nonrelativistic Hamiltonian of a particle of charge Q is given by

$$H = \frac{1}{2m} \left(\mathbf{p} - \frac{Q}{c} \mathbf{A}(\mathbf{x}, t) \right) \cdot \left(\mathbf{p} - \frac{Q}{c} \mathbf{A}(\mathbf{x}, t) \right) + Q\phi(\mathbf{x}, t). \quad (1.1.27)$$

Considered in conjunction with the Schrödinger equation, Eq. (1.1.1), the time rate of change of the charge density, $\rho(\mathbf{x}, t) = Q\Psi^*(\mathbf{x}, t)\Psi(\mathbf{x}, t)$, is given by

$$i\hbar \frac{\partial}{\partial t} \rho(\mathbf{x}, t) = Q\Psi^*(\mathbf{x}, t) \left[\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{Q}{c} \mathbf{A}(\mathbf{x}, t) \right) \cdot \left(\frac{\hbar}{i} \nabla - \frac{Q}{c} \mathbf{A}(\mathbf{x}, t) \right) + Q\phi \right] \Psi(\mathbf{x}, t) - h.c., \quad (1.1.28)$$

where *h.c.* denotes the Hermitian conjugate. This may be rewritten as

$$\begin{aligned} \frac{\partial \rho(\mathbf{x}, t)}{\partial t} = & -\nabla \cdot \left\{ \frac{\hbar Q}{2m} \left[(i\nabla \Psi^*(\mathbf{x}, t)) \Psi(\mathbf{x}, t) - \Psi^*(\mathbf{x}, t) (i\nabla \Psi(\mathbf{x}, t)) \right] \right. \\ & \left. - \frac{Q^2}{mc} \mathbf{A}(\mathbf{x}, t) \Psi^*(\mathbf{x}, t) \Psi(\mathbf{x}, t) \right\}. \end{aligned} \quad (1.1.29)$$

Considered with the equation of continuity for the conserved (normalized) charge-probability density, $\rho(\mathbf{x}, t)$,

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} = -\nabla \cdot \mathbf{J}(\mathbf{x}, t), \quad (1.1.30)$$

we may identify the charge-current density, $\mathbf{J}(\mathbf{x}, t)$,

$$\mathbf{J}(\mathbf{x}, t) = \frac{\hbar Q}{2m} \left[\Psi^*(\mathbf{x}, t) \left(\frac{1}{i} \nabla \Psi(\mathbf{x}, t) \right) - \left(\frac{1}{i} \nabla \Psi^*(\mathbf{x}, t) \right) \Psi(\mathbf{x}, t) \right] - \frac{Q^2}{mc} \mathbf{A}(\mathbf{x}, t) \Psi^*(\mathbf{x}, t) \Psi(\mathbf{x}, t). \quad (1.1.31)$$

It is important to note that $\mathbf{J}$ is invariant under a gauge transformation, $\mathbf{A}(\mathbf{x}, t) \rightarrow \mathbf{A}'(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}, t) + \nabla f(\mathbf{x}, t)$ and $\phi(\mathbf{x}, t) \rightarrow \phi'(\mathbf{x}, t) = \phi(\mathbf{x}, t) - \frac{1}{c} \frac{\partial}{\partial t} f(\mathbf{x}, t)$, taken jointly with the phase transformation,

$$\Psi(\mathbf{x}, t) \rightarrow e^{i Q f(\mathbf{x}, t)/\hbar c} \Psi(\mathbf{x}, t). \quad (1.1.32)$$

This phase change describes the transformation that wave functions must undergo in conjunction with an electromagnetic gauge transformation to preserve the gauge invariance of the physical quantities in quantum mechanics.

In dealing with two particles, we have a Hamiltonian that depends on the coordinates and momenta of both particles,

$$H \longrightarrow H(\mathbf{x}_1, \frac{\hbar}{i} \nabla_1; \mathbf{x}_2, \frac{\hbar}{i} \nabla_2). \quad (1.1.33)$$

The wave function also depends on both coordinates,

$$\Psi \longrightarrow \Psi(\mathbf{x}_1, \mathbf{x}_2, t). \quad (1.1.34)$$

Correspondingly, Hermitian operators involving two particles are employed,

$$\Theta \longrightarrow \Theta(\mathbf{x}_1, \frac{\hbar}{i} \nabla_1; \mathbf{x}_2, \frac{\hbar}{i} \nabla_2), \quad (1.1.35)$$

and their eigenfunctions involve both coordinates,

$$\phi \longrightarrow \phi(\mathbf{x}_1, \mathbf{x}_2). \quad (1.1.36)$$

Similar extensions are made for N particles. Continuing for the moment with two particles, the quantum mechanical principle of indistinguishability for similar particles must be satisfied. This means that the state obtained by the interchange of the coordinates of any two identical particles must be physically indistinguishable from the original state and physically equivalent to it. Therefore, they can only differ by a constant phase factor since the probability density and current are unaffected:

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, t) = e^{i\alpha} \Psi(\mathbf{x}_2, \mathbf{x}_1, t). \quad (1.1.37)$$

Interchanging the particle coordinates a second time,

$$\Psi(\mathbf{x}_2, \mathbf{x}_1, t) = e^{i\alpha} \Psi(\mathbf{x}_1, \mathbf{x}_2, t), \quad (1.1.38)$$

must yield the original wave function, so it is clear that $e^{2i\alpha} = 1$, whence

$$e^{i\alpha} = \pm 1 \quad \text{and} \quad \Psi(\mathbf{x}_1, \mathbf{x}_2, t) = \pm \Psi(\mathbf{x}_2, \mathbf{x}_1, t). \quad (1.1.39)$$

The upper sign (+) reflects a symmetric state and particles having such wave functions will be seen to obey Bose–Einstein statistics and are called “Bosons.” The lower sign (–) reflects an antisymmetric state. The particles in this case will be seen to obey Fermi–Dirac statistics and are called “Fermions.”

If the particles do not interact, it is possible to solve the time-independent Schrödinger energy eigenvalue equation easily by separation of variables, $H \rightarrow h_1 + h_2$, since each part of the Hamiltonian depends only on one particle’s coordinates:

$$\left[h_1 \left(\mathbf{x}_1, \frac{\hbar}{i} \nabla_1 \right) + h_2 \left(\mathbf{x}_2, \frac{\hbar}{i} \nabla_2 \right) \right] \phi_E(\mathbf{x}_1, \mathbf{x}_2) = E \phi_E(\mathbf{x}_1, \mathbf{x}_2), \quad (1.1.40)$$

with $\phi_E(\mathbf{x}_1, \mathbf{x}_2) = \phi_{E_1}(\mathbf{x}_1) \phi_{E_2}(\mathbf{x}_2)$ and $E_1 + E_2 = E$. The symmetry/antisymmetry requirements of the Pauli exclusion principle may be imposed on these separated solutions to obtain the properly normalized two-particle energy eigenfunctions in the symmetrical/antisymmetrical cases in the form

$$\phi_E(\mathbf{x}_1, \mathbf{x}_2) = \frac{[\phi_{E_1}(\mathbf{x}_1) \phi_{E_2}(\mathbf{x}_2) \pm \phi_{E_1}(\mathbf{x}_2) \phi_{E_2}(\mathbf{x}_1)]}{\sqrt{2}}. \quad (1.1.41)$$

Generalizing the non-interacting case to N particles, we similarly obtain non-interacting N -particle energy eigenfunctions as

$$\phi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \left\{ \begin{array}{c} \det \\ \text{perm} \end{array} \right\} \begin{vmatrix} \phi_{E_1}(\mathbf{x}_1) \phi_{E_1}(\mathbf{x}_2) \cdots \phi_{E_1}(\mathbf{x}_N) \\ \phi_{E_2}(\mathbf{x}_1) \phi_{E_2}(\mathbf{x}_2) \cdots \phi_{E_2}(\mathbf{x}_N) \\ \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \\ \phi_{E_n}(\mathbf{x}_1) \phi_{E_n}(\mathbf{x}_2) \cdots \phi_{E_n}(\mathbf{x}_N) \end{vmatrix}, \quad (1.1.42)$$

with the energy eigenvalue $\sum_{i=1}^N E_i = E$. Here “det” and “perm” stand for determinant and permanent, respectively, and the permanent is the same linear combination of products of wave functions as the determinant, except that all signs are positive. In the antisymmetric case (Fermions) this is called the “Slater determinant,” and it vanishes if any two “occupied states,” ϕ_{E_i} and ϕ_{E_j} , are the same, so that no two (or more) Fermi particles can be in the same state. This is the Pauli exclusion principle for Fermions. Bosons are not subject to such a restriction on the occupation of states.

Note that if there is interaction, so that the eigenfunctions are not separable, we can still take a two-particle energy eigenfunction, $\phi_E(\mathbf{x}_1, \mathbf{x}_2)$, and symmetrize/antisymmetrize it as follows:

$$\frac{[\phi_E(\mathbf{x}_1, \mathbf{x}_2) \pm \phi_E(\mathbf{x}_2, \mathbf{x}_1)]}{\sqrt{2}}. \quad (1.1.43)$$

This is readily extended to N particles.

1.2 Dirac Notation

We will now redescribe wave functions in terms of abstract state vectors, introducing Dirac notation.⁴⁻⁷ A single-particle wave function $\Psi(\mathbf{x})$ can be viewed as a column state vector or “function vector” (suppressing t -dependence),

$$\Psi(\mathbf{x}) \rightarrow \begin{pmatrix} \Psi(\mathbf{x}_1) \\ \Psi(\mathbf{x}_2) \\ \vdots \\ \Psi(\mathbf{x}_N) \\ \vdots \end{pmatrix}, \quad (1.2.1)$$

in a space having a continuum of dimensions, one for each value of $\mathbf{x}$, with $\Psi(\mathbf{x}_i)$ being the i^{th} component of the vector. Denoting the corresponding abstract vector by $|\Psi\rangle$, termed a “ket” by Dirac,^{4,5} and its adjoint $|\Psi\rangle^+ = \langle\Psi|$ (Dirac’s “bra”), we have scalar (dot “inner”) products of the type

$$\langle\Psi'| \cdot |\Psi\rangle \equiv \langle\Psi'|\Psi\rangle, \quad (1.2.2)$$

which form “bra-ket” structures, or “brackets.” In these terms the i^{th} component of $|\Psi\rangle$ can be written as

$$\langle\mathbf{x}_i|\Psi\rangle \equiv \Psi(\mathbf{x}_i), \quad (1.2.3)$$

where the unit vector in the i^{th} coordinate direction of our function vector space, the direction associated with $\mathbf{x}_i$, is denoted by $|\mathbf{x}_i\rangle$, an eigenvector of the position operator $\mathbf{X}$ with eigenvalue $\mathbf{x}_i$. We call this the “position” representation of the state vector $|\Psi\rangle$. Since the unit vectors $|\mathbf{x}_i\rangle$ along the $\mathbf{x}_i$ -coordinate directions represent mutually perpendicular unit vectors along the directions of mutually independent coordinate axes, the scalar product is given by

$$\langle\mathbf{x}_i|\mathbf{x}_j\rangle \Rightarrow \delta_{ij}, \quad (1.2.4)$$

and for the continuum of dimensions involved, this means that δ_{ij} is to be understood as a Dirac delta function,

$$\langle\mathbf{x}_i|\mathbf{x}_j\rangle = \delta^{(3)}(\mathbf{x}_i - \mathbf{x}_j). \quad (1.2.5)$$

Henceforth, we will drop superfluous subscripts on $\mathbf{x}$, understanding that each value of $\mathbf{x}$ indexes a separate orthogonal direction in the function vector space.

In terms of bras and kets, the completeness relation, $\Psi(\mathbf{x}) = \sum_r C_r \phi_r(\mathbf{x})$, becomes $\langle\mathbf{x}|\Psi\rangle = \sum_r C_r \langle\mathbf{x}|r\rangle$, so that $|\Psi\rangle = \sum_r C_r |r\rangle$. Alternatively, completeness can be expressed as (note that $\langle\mathbf{x}'|r\rangle^* = (\langle\mathbf{x}'|r\rangle)^+ = \langle r|\mathbf{x}'\rangle$ since the adjoint of a product is the product of the adjoints individually in reverse order, and $|r\rangle^+ \equiv \langle r|$, etc.):

$$\begin{aligned}
\delta^{(3)}(\mathbf{x} - \mathbf{x}') &= \sum_r \phi_r^*(\mathbf{x}') \phi_r(\mathbf{x}) = \sum_r \langle \mathbf{x}' | r \rangle^* \langle \mathbf{x} | r \rangle, \\
&= \sum_r \langle \mathbf{x} | r \rangle \langle r | \mathbf{x}' \rangle,
\end{aligned} \tag{1.2.6}$$

and since

$$\langle \mathbf{x} | \mathbf{x}' \rangle = \delta^{(3)}(\mathbf{x} - \mathbf{x}') = \langle \mathbf{x} | \left(\sum_r |r\rangle \langle r| \right) | \mathbf{x}' \rangle, \tag{1.2.7}$$

we have the completeness relation as a sum of ket-bra “outer-product” structures as

$$\sum_r |r\rangle \langle r| = \mathbf{I}, \tag{1.2.8}$$

where $\mathbf{I}$ is the identity operator. In this form of the completeness relation, the sum is extended over all r -state vectors of the complete set, which means integration in the case of a continuum,

$$\int d^{(3)}\mathbf{x} |\mathbf{x}\rangle \langle \mathbf{x}| = \mathbf{I}. \tag{1.2.9}$$

The ket-bra outer-product structures involved here are *not* scalar-dot products, but are operators in the function vector space. They involve *no* multiplication between the ket and bra internally, but the ket can be dot multiplied to the left and the bra can be dot multiplied to the right.

Furthermore, the orthogonality relation is

$$\begin{aligned}
\int d^{(3)}\mathbf{x} \phi_r^*(\mathbf{x}) \phi_s(\mathbf{x}) &= \int d^{(3)}\mathbf{x} \langle \mathbf{x} | r \rangle^* \langle \mathbf{x} | s \rangle, \\
&= \langle r | \left[\int d^{(3)}\mathbf{x} |\mathbf{x}\rangle \langle \mathbf{x}| \right] | s \rangle, \\
&= \langle r | \mathbf{I} | s \rangle = \langle r | s \rangle = \delta_{rs}.
\end{aligned} \tag{1.2.10}$$

(Again, in the case of a continuum, δ_{rs} is supplanted by a Dirac delta function.) Finally, we note that C_r is given by

$$\begin{aligned}
C_r &= \int d^{(3)}\mathbf{x} \phi_r^*(\mathbf{x}) \Psi(\mathbf{x}), \\
&= \int d^{(3)}\mathbf{x} \langle r | \mathbf{x} \rangle \langle \mathbf{x} | \Psi \rangle, \\
&= \langle r | \left[\int d^{(3)}\mathbf{x} |\mathbf{x}\rangle \langle \mathbf{x}| \right] | \Psi \rangle,
\end{aligned} \tag{1.2.11}$$

or,

$$C_r = \langle r | \Psi \rangle, \quad (1.2.12)$$

which could have been obtained directly from the results above using

$$|\Psi\rangle = \sum_{r'} C_{r'} |r'\rangle \quad (1.2.13)$$

and

$$\langle r | r' \rangle = \delta_{rr'} = \langle r' | r \rangle, \quad (1.2.14)$$

since

$$\langle r | \Psi \rangle = \sum_{r'} C_{r'} \langle r | r' \rangle = \sum_{r'} C_{r'} \delta_{rr'} = C_r. \quad (1.2.15)$$

(Restoring time dependence, $|\Psi\rangle \rightarrow |\Psi(t)\rangle$ and $C_{r'} \rightarrow C_{r'}(t)$.)

Having identified the identity operator as a ket-bra structure, $\mathbf{I} = \sum_r |r\rangle\langle r|$, we now examine a more general operator structure corresponding to a matrix having matrix elements $M_{rr'}$:

$$\mathbf{M} = \sum_r \sum_{r'} |r\rangle M_{rr'} \langle r'|. \quad (1.2.16)$$

Again, there is no internal multiplication between the ket and bra of the outer product, but the ket can dot multiply to the left and the bra can dot multiply to the right. We will show below that with the above rules for multiplication, the operator $\mathbf{M}$ has operator multiplication properties that correspond exactly to those of the matrix with elements $M_{rr'}$. Consider first,

$$\mathbf{M}|r'\rangle = \sum_r \sum_{r''} |r\rangle M_{rr''} \langle r'' | r' \rangle = \sum_r |r\rangle M_{rr'} \quad (1.2.17)$$

and

$$\langle r | \mathbf{M} | r' \rangle = \sum_{r''} \langle r | r'' \rangle M_{r''r'} = M_{rr'}, \quad (1.2.18)$$

where the orthogonality relation, $\langle r'' | r' \rangle = \delta_{r''r'}$, has been used in both stages. This is a very convenient way of representing an operator and it justifies Dirac's bra-ket notation since the matrix element of $\mathbf{M}$ ($M_{rr'}$) is here seen to be the bracket ("bra-ket") of the abstract operator $\mathbf{M}$ between the bra $\langle r |$ and the ket $|r'\rangle$. A final verification may be obtained by noting that we simply have an identity, since

$$\begin{aligned} \mathbf{M} &= \sum_r \sum_{r'} |r\rangle \langle r | \mathbf{M} | r' \rangle \langle r'| = \left[\sum_r |r\rangle \langle r| \right] \mathbf{M} \left[\sum_{r'} |r'\rangle \langle r'| \right] \\ &= \mathbf{I} \cdot \mathbf{M} \cdot \mathbf{I} = \mathbf{M}. \end{aligned} \quad (1.2.19)$$

Dirac's ket-bra operators are just dyadic operators, such as those that have been used in electromagnetic theory for a long time.⁸⁻¹⁰

In regard to the implications of this for the position representation, where matrix elements are usually written as

$$M_{rr'} = \int d^{(3)}\mathbf{x} \phi_r^*(\mathbf{x}) M(\mathbf{x}, \frac{\hbar}{i} \nabla) \phi_{r'}(\mathbf{x}), \quad (1.2.20)$$

or, alternatively,

$$\langle r | \mathbf{M} | r' \rangle = \langle r | \int d^{(3)}\mathbf{x} | \mathbf{x} \rangle M(\mathbf{x}, \frac{\hbar}{i} \nabla) \langle \mathbf{x} | r' \rangle, \quad (1.2.21)$$

we have

$$\mathbf{M} = \int d^{(3)}\mathbf{x} | \mathbf{x} \rangle M(\mathbf{x}, \frac{\hbar}{i} \nabla) \langle \mathbf{x} |. \quad (1.2.22)$$

However,

$$\begin{aligned} \langle \mathbf{x}' | \mathbf{M} | \mathbf{x}'' \rangle &= \int d^{(3)}\mathbf{x} \langle \mathbf{x}' | \mathbf{x} \rangle M(\mathbf{x}, \frac{\hbar}{i} \nabla) \langle \mathbf{x} | \mathbf{x}'' \rangle \\ &= \int d^{(3)}\mathbf{x} \delta^{(3)}(\mathbf{x}' - \mathbf{x}) M(\mathbf{x}, \frac{\hbar}{i} \nabla) \delta^{(3)}(\mathbf{x} - \mathbf{x}''), \end{aligned} \quad (1.2.23)$$

so that

$$M_{\mathbf{x}'\mathbf{x}''} = \delta^{(3)}(\mathbf{x}' - \mathbf{x}'') M(\mathbf{x}', \frac{\hbar}{i} \nabla') \quad (1.2.24)$$

is diagonal in position representation. Applying this to the eigenfunction equation,

$$\Theta(\mathbf{x}, \frac{\hbar}{i} \nabla) \phi_r(\mathbf{x}) = \lambda_r \phi_r(\mathbf{x}), \quad (1.2.25)$$

we write:

$$\int d^{(3)}\mathbf{x}' \Theta(\mathbf{x}, \frac{\hbar}{i} \nabla) \delta^{(3)}(\mathbf{x}' - \mathbf{x}) \phi_r(\mathbf{x}') = \lambda_r \langle \mathbf{x} | r \rangle. \quad (1.2.26)$$

Using the fact that $\Theta_{\mathbf{x}\mathbf{x}'} = \langle \mathbf{x} | \Theta | \mathbf{x}' \rangle$ is diagonal in position representation, we have

$$\int d^{(3)}\mathbf{x}' \langle \mathbf{x} | \Theta | \mathbf{x}' \rangle \langle \mathbf{x}' | r \rangle = \langle \mathbf{x} | \Theta | r \rangle = \lambda_r \langle \mathbf{x} | r \rangle, \quad (1.2.27)$$

since $\int d^{(3)}\mathbf{x}' | \mathbf{x}' \rangle \langle \mathbf{x}' | = \mathbf{I}$ is the identity operator. Thus, the eigenvector equation is just

$$\Theta | r \rangle = \lambda_r | r \rangle. \quad (1.2.28)$$

Similarly, for the Schrödinger equation,

$$H(\mathbf{x}, \frac{\hbar}{i}\nabla)\Psi(\mathbf{x}, t) = i\hbar\frac{\partial\Psi(\mathbf{x}, t)}{\partial t} \quad (1.2.29)$$

or,

$$\langle\mathbf{x}|H|\Psi\rangle = i\hbar\langle\mathbf{x}|\frac{\partial\Psi}{\partial t}\rangle, \quad (1.2.30)$$

from which

$$H|\Psi\rangle = i\hbar\frac{\partial|\Psi\rangle}{\partial t}. \quad (1.2.31)$$

It is, of course, important to verify that the multiplication properties of operators written as

$$\mathbf{M} = \sum_r \sum_{r'} |r\rangle M_{rr'} \langle r'| \quad (1.2.32)$$

just replicate the matrix multiplication properties. Consider a product of two such operators,

$$\mathbf{M} \cdot \mathbf{N} = \sum_r \sum_{r'} \sum_{r''} \sum_{r'''} |r\rangle M_{rr'} \langle r'| \cdot |r''\rangle N_{r''r'''} \langle r'''|. \quad (1.2.33)$$

Using the orthogonality relation, $\langle r'|r''\rangle = \delta_{r'r''}$, we have

$$\mathbf{M} \cdot \mathbf{N} = \sum_r \sum_{r'} \sum_{r'''} |r\rangle M_{rr'} N_{r'r'''} \langle r'''|. \quad (1.2.34)$$

Now (we write $r''' \equiv r^{iv}$, etc.):

$$\begin{aligned} (\mathbf{M} \cdot \mathbf{N})_{r^{iv}, r^v} &= \langle r^{iv} | \mathbf{M} \cdot \mathbf{N} | r^v \rangle, \\ &= \sum_r \sum_{r'} \sum_{r'''} \langle r^{iv} | \cdot | r \rangle M_{rr'} N_{r'r'''} \langle r''' | \cdot | r^v \rangle, \\ &= \sum_r \sum_{r'} \sum_{r'''} \delta_{r^{iv}r} M_{rr'} N_{r'r'''} \delta_{r'''r^v}, \\ &= \sum_{r'} M_{r^{iv}r'} N_{r'r^v}, \end{aligned} \quad (1.2.35)$$

which properly follows the rule for matrix multiplication. Dirac's introduction of dyadic notation facilitates many derivations and calculations in quantum theory, and greatly clarifies many aspects of quantum mechanics. As we will see, Schwinger has introduced further interpretation of the dyadic structures, which yield "second quantization" in a remarkably simple way.

1.3 Complete Sets of Commuting Observables, Representations and Transformation Theory

Taking a broader view of Eq. (1.2.28), we may understand Θ to stand for a complete set of commuting Hermitian operators, $A = \{A_1, A_2, \dots, A_l\}$, corresponding to a complete set of compatible observables^{2,4,7} (compatible in the sense that they can be measured precisely simultaneously). Such completeness means that all the members of the set have common eigenvectors, $|a'\rangle$, which are not degenerate, with a corresponding set of eigenvalues, $a' \rightarrow \{a'_i\}$, that uniquely define a state of maximum information permitted by the laws of quantum mechanics. Moreover, any other operator of the system that is compatible/commutative with $A = \{A_i\}$ is necessarily a function of the set $\{A_i\}$; and any other independent property of the system is incompatible/non-commutative with some member(s) of the set $\{A_i\}$. Thus, we understand A to represent a complete set of compatible observables/operators:

$$\Theta \rightarrow A = \{A_1, A_2, \dots, A_l\}, \quad (1.3.1)$$

with $[A_i, A_j] = 0$, ($i = 1 \dots l; j = 1 \dots l$), and

$$A|a'\rangle = a'|a'\rangle, \quad (1.3.2)$$

in the sense that

$$A_i|a'\rangle = a'_i|a'\rangle \quad (i = 1, 2, \dots, l) \quad (1.3.3)$$

describes the set of common eigenvectors of the complete set of commuting operators A , corresponding to the compatible observables that uniquely define a non-degenerate state $|a'\rangle$ of the system. The adjoint of such a ket $|a'\rangle^+ = \langle a'|$ is a bra-state, and the orthonormality of two such eigenstates of A , $|a'\rangle$ and $|a''\rangle$, is given by

$$\langle a'|a''\rangle = \delta_{a'a''}, \quad (1.3.4)$$

with completeness described by

$$\sum_{a'} |a'\rangle \langle a'| = \mathbf{I}. \quad (1.3.5)$$

Moreover, in summary, the Schrödinger equation is

$$H|\Psi(t)\rangle = i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} \quad (1.3.6)$$

and $|\Psi(t)\rangle$ may be expanded in the eigenvectors of A as

$$|\Psi(t)\rangle = \sum_{a'} C_{a'}(t) |a'\rangle, \quad (1.3.7)$$

where the coefficient $C_{a'}(t)$ is given by

$$C_{a'}(t) = \langle a' | \Psi(t) \rangle \equiv \Psi(a', t) \quad (1.3.8)$$

and is called “the state (or wave function) $|\Psi(t)\rangle$ in an A -representation,” $\Psi(a', t)$. Also, an operator $\mathbf{M}$ having matrix elements $\mathbf{M}_{a'a''} = \langle a' | \mathbf{M} | a'' \rangle$ in an A -representation has the form

$$\mathbf{M} = \sum_{a'} \sum_{a''} |a'\rangle \mathbf{M}_{a'a''} \langle a''|. \quad (1.3.9)$$

This constitutes the description of an A -representation with basis vectors $|a'\rangle$.

We could equally well choose a different complete compatible and commuting set of observable Hermitian operators $B = \{B_1, B_2, \dots, B_l\}$ having a complete set of common eigenvectors $|b'\rangle$,

$$B |b'\rangle = b' |b'\rangle, \quad (1.3.10)$$

and adjoints $|b'\rangle^+ = \langle b'|$, with orthogonality given by $\langle b' | b'' \rangle = \delta_{b'b''}$. In this case we would have the B -representation with basis vectors $|b'\rangle$, $\langle b' | \Psi(t) \rangle$ as the state $|\Psi(t)\rangle$ in the B -representation, $\Psi(b', t)$, and $\mathbf{M}_{b'b''} = \langle b' | \mathbf{M} | b'' \rangle$ as the matrix elements of $\mathbf{M}$ in the B -representation. It is straightforward to transform from one representation, or basis, to another. Consider $|\Psi\rangle$ in the A -representation,

$$\Psi(a') = \langle a' | \Psi \rangle = \langle a' | \mathbf{I} | \Psi \rangle, \quad (1.3.11)$$

and insert the identity in the B -representation,

$$\mathbf{I} = \sum_{b'} |b'\rangle \langle b'|, \quad (1.3.12)$$

to obtain

$$\Psi(a') = \sum_{b'} \langle a' | b' \rangle \langle b' | \Psi \rangle = \sum_{b'} \langle a' | b' \rangle \Psi(b'). \quad (1.3.13)$$

Furthermore,

$$\mathbf{M}_{a'a''} = \langle a' | \mathbf{M} | a'' \rangle = \langle a' | \mathbf{I} \cdot \mathbf{M} \cdot \mathbf{I} | a'' \rangle, \quad (1.3.14)$$

and again writing $\mathbf{I}$ in the B -representation, or basis, we have

$$\begin{aligned} \mathbf{M}_{a'a''} &= \sum_{b'} \sum_{b''} \langle a' | b' \rangle \langle b' | \mathbf{M} | b'' \rangle \langle b'' | a'' \rangle \\ &= \sum_{b', b''} \langle a' | b' \rangle \mathbf{M}_{b'b''} \langle b'' | a'' \rangle. \end{aligned} \quad (1.3.15)$$

Eqs. (1.3.13) and (1.3.15) are the fundamental relations of transformation theory. Note that while there is orthogonality among the eigenvectors $|a'\rangle$, and, separately, there is

orthogonality among the eigenvectors $|b'\rangle$, they are *not* mutually orthogonal, $\langle a' | b' \rangle \neq 0$, because they are eigenvectors of different complete commuting operator sets. In fact, the $\langle a' | b' \rangle$ are the “transformation” functions that facilitate the change of basis described in Eqns. (1.3.13) and (1.3.15). Finally, it should be noted that any Hermitian operator $\mathbf{M}$ can be brought to diagonal form by transformation to the basis of its eigenvectors, $|m'\rangle$, since the eigenvalue equation, $\mathbf{M}|m'\rangle = m'|m'\rangle$, from which

$$\mathbf{M}_{mm'} = \langle m | \mathbf{M} | m' \rangle = m' \langle m | m' \rangle = m \delta_{mm'}. \quad (1.3.16)$$

1.4 Schwinger Measurement Symbols

It is sometimes useful to construct operators in a “mixed” representation by writing

$$\mathbf{M} = \mathbf{I} \cdot \mathbf{M} \cdot \mathbf{I}, \quad (1.4.1)$$

where the first identity is written in the A -representation and the second identity is written in the B -representation, obtaining

$$\begin{aligned} \mathbf{M} &= \sum_{a'} |a'\rangle \langle a'| \cdot \mathbf{M} \cdot \sum_{b'} |b'\rangle \langle b'| \\ &= \sum_{a', b'} |a'\rangle \mathbf{M}_{a'b'} \langle b'|, \end{aligned} \quad (1.4.2)$$

where

$$\mathbf{M}_{a'b'} = \langle a' | \mathbf{M} | b' \rangle \quad (1.4.3)$$

is the “mixed” matrix element of $\mathbf{M}$. Also, Eq. (1.4.2) employs mixed dyadic operators, called “measurement symbols,” which are defined as

$$\mathcal{M}(a', b') \equiv |a'\rangle \langle b'|, \quad (1.4.4)$$

such that

$$\mathbf{M} = \sum_{a', b'} \mathbf{M}_{a'b'} \mathcal{M}(a', b') = \sum_{a', b'} \langle a' | \mathbf{M} | b' \rangle \mathcal{M}(a', b'). \quad (1.4.5)$$

Considering the action of the measurement symbol $\mathcal{M}(a', b')$ on an arbitrary state,

$$|\Psi\rangle = \sum_{b''} |b''\rangle \langle b'' | \Psi \rangle = \sum_{b''} |b''\rangle \Psi(b''), \quad (1.4.6)$$

we have

$$\mathcal{M}(a', b') |\Psi\rangle = |a'\rangle \sum_{b''} \langle b' | b'' \rangle \Psi(b'') = |a'\rangle \Psi(b'), \quad (1.4.7)$$

since $\langle b' | b'' \rangle = \delta_{b'b''}$. Thus, the action of $\mathcal{M}(a', b')$ on $|\Psi\rangle$ may be described as a two-step process:

1. It selects the component of $|\Psi\rangle$ associated with $|b'\rangle$, that is, it selects the probability amplitude for $|\Psi\rangle$ to be found in $|b'\rangle$ if a B -measurement were to be made.
2. It eliminates the state $|b'\rangle$, replacing it by $|a'\rangle$, carrying along the original amplitude $\Psi(b')$.

This has been interpreted by Schwinger in the following way:^{11,12}

“ $\mathcal{M}(a', b')$ acts as an operator representing a selective measurement that changes the state upon which it acts. It selects only systems in the state $|b'\rangle$ out of the totality of impinging system states, rejecting all others; following this it emits these systems in the state $|a'\rangle$. The measurement itself entails an uncontrollable disturbance, which is beyond our scrutiny; it is an indivisible act about which we know only the initial and final states of the system, that is to say that the first stage selects systems in the state $|b'\rangle$ and that the last stage produces them in the state $|a'\rangle$. There is no physical meaning to any attempt to trace the history of the measurement process in detail, since no such information is available. However, so long as we do not interfere with the initial and final states, we may imagine this measurement process to take part in two stages associated with the interposition of a non-physical *null* state as an intermediary. We call this imagined *null* state 0 and write

$$\mathcal{M}(a', b') = \mathcal{M}(a', 0)\mathcal{M}(0, b').”^{11} \quad (1.4.8)$$

(Note that $\mathcal{M}(0, a') = \mathcal{M}^+(a', 0)$.) In accordance with this interpretation, $\mathcal{M}(0, b')$ represents the measurement process that selects a system in the state $|b'\rangle$, and emits it in the limbo state, called the *null* state (which is *not* any of the eigenstates $|a'\rangle$ or $|b'\rangle$ discussed above). This may be described as the *annihilation* of a system in the state $|b'\rangle$. Correspondingly, in this interpretive scheme, the ensuing action of $\mathcal{M}(a', 0)$ then *creates* (out of the limbo *null* state) and emits a system in the state $|a'\rangle$ (following its selection from the *null* state). This joint action of the operators $\mathcal{M}(a', 0)\mathcal{M}(0, b')$ thus has the same effect as $\mathcal{M}(a', b')$, which we can therefore describe as *annihilating* a system in $|b'\rangle$, along with the *creation* of a system in state $|a'\rangle$.^{12–14} This will be considered further in a many-particle context.

1.5 Chapter 1 Problems

P.1.1. Eq. (1.1.10) says that $[L_1, L_2] \neq 0$. Prove that $[L_i, \mathbf{L}^2] = 0$.

P.1.2. Prove that L_3 generates infinitesimal rotations about the 3-axis.

P.1.3. Show that:

- (a) $[A, BC] = B[A, C] + [A, B]C$ for quantum operators A,B,C, and that
- (b) $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$.

P.1.4. Consult the literature to discuss the relations between

- (a) e^{A+B} and $e^A e^B$, also

- (b) $\frac{de^{C(t)}}{dt}$ and $e^{C(t)} \frac{dC(t)}{dt}$.

P.1.5. Consider a one-dimensional (1D) simple harmonic oscillator with the Hamiltonian $H = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}$, where q, p obey canonical commutation relations:

- (a) Determine its eigenvalues, E_n , and eigenfunctions, ϕ_n , in position (q) representation.
- (b) Defining operators

$$c = \sqrt{\frac{m\omega}{2\hbar}}(q + ip/m\omega),$$

$$c^+ = \sqrt{\frac{m\omega}{2\hbar}}(q - ip/m\omega),$$

write H in terms of c, c^+ , and determine their commutation relations with each other. Show that $c^+ c$ commutes with H , and denoting their common eigenvectors by $\phi_n \rightarrow |n\rangle$, prove that

$$(c^+ c) |n\rangle = (\lambda_n + 1) c^+ |n\rangle$$

$$(\lambda_n = n = 0, 1, 2 \dots),$$

where $(c^+ c) |n\rangle = \lambda_n |n\rangle$, so that c^+ has the interpretation of a “raising” operator. Show that c has the corresponding interpretation of a “lowering” operator.

- (c) If we start with recognition that the lowest λ_n eigenvalue is $\lambda_0 = 0$ (and $c|0\rangle = 0$, correspondingly), show that the “ladder” procedure in the sequential application of c^+ operators yields the n^{th} eigenstate as $|n\rangle = N_n (c^+)^n |0\rangle$. Determine the normalization constant N_n .

P.1.6. Verify Eqns. (1.1.23) and (1.1.24).

P.1.7. On the right-hand side of Eq. (1.1.28), why is $(-h.c.; \text{minus Hermitian conjugate})$ appropriate?

P.1.8. Verify Eq. (1.1.31).

P.1.9. Prove that Eq. (1.1.32) correctly describes the behavior of the wave function under a gauge transformation.

P.1.10. What is the relation between an eigenfunction of energy in a position representation and the corresponding position eigenfunction in an energy representation?

P.1.11. Verify that $M|\Psi\rangle$ and $\langle\Psi|M$ (where M is given by Eq. (1.2.16)). Follow the usual multiplication rules between a matrix and a state vector.

- P.1.12.** Prove that Dirac's representation of operators in terms of ket-bra ($|i\rangle\langle j|$) structures is equivalent to the dyadic ($\hat{e}_i, \hat{e}_j^+$) notation of electromagnetic theory (see, for example, Reference 10 in Section 1.6, pp. 62–77), having the same multiplication and transformation properties under a change of basis.
- P.1.13.** A projection operator P has the property that $P^2 = P$. Show that for any subset m of dyadics of the type $|a'_i\rangle\langle a'_i|$, the sum $\sum_{i=1}^m |a'_i\rangle\langle a'_i|$ has this property.
- P.1.14.** Prove the identity for a variation δ of an operator X :

$$\delta(\log \det X) = \text{tr}(X^{-1} \delta X).$$

- P.1.15.** Prove the following identity for Pauli spin matrices $\boldsymbol{\sigma} = \sigma_1 \hat{i} + \sigma_2 \hat{j} + \sigma_3 \hat{k}$ and two arbitrary vectors $\mathbf{a}, \mathbf{b}$:

$$(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b} + i\boldsymbol{\sigma} \cdot \mathbf{a} \times \mathbf{b},$$

and if $\hat{n}$ is an arbitrary unit vector, show that

$$(\boldsymbol{\sigma} \cdot \hat{n})^2 = 1.$$

- P.1.16.** Construct the unitary similarity transformation that diagonalizes the matrix $\boldsymbol{\sigma} \cdot \mathbf{H}$.
- P.1.17.** Hamilton's generalization of pure imaginaries $\underline{i}, \underline{j}, \underline{k}$ may be defined as:
 $\underline{i} = -i\sigma_1, \underline{j} = -i\sigma_2, \underline{k} = -i\sigma_3$.
 Show that $\underline{i}, \underline{j}, \underline{k}$ obey the following multiplication rules:
 (a) $\underline{i}^2 = \underline{j}^2 = \underline{k}^2 = -I$
 (b) $\underline{i}\underline{j} = -\underline{j}\underline{i} = \underline{k}; \underline{j}\underline{k} = -\underline{k}\underline{j} = \underline{i};$ and $\underline{k}\underline{i} = -\underline{i}\underline{k} = \underline{j}$.
- P.1.18.** A quaternion Q is defined as:
 $Q \equiv t + \underline{i}x + \underline{j}y + \underline{k}z$,
 where t, x, y and z are *real* numbers (notice that all real numbers are quaternions). Prove that:
 (a) If Q_1 and Q_2 are quaternions, then $(Q_1 + Q_2)$ and $(Q_1 \cdot Q_2)$ are also quaternions.
 (b) $Q^+ Q = \text{real number}$, where Q^+ is called the “complex conjugate” of the quaternion Q and is given by $Q^+ = t - \underline{i}x - \underline{j}y - \underline{k}z$, with Q as above (notice that Q^+ is also a quaternion).
 (c) For every quaternion Q there exists another quaternion Q^{-1} such that $Q^{-1} Q = Q Q^{-1} = 1$.
- P.1.19.** The Hamiltonian of a charged particle in a magnetic field $\mathbf{B}$ given in Eq. (1.1.27) neglects a “Zeeman spin-splitting” term, $\bar{\mu}_0 \boldsymbol{\sigma} \cdot \mathbf{B}$. Consider the case in which all *other* electromagnetic field effects are negligible and solve the following equation for the 2×2 matrix $G(\mathbf{p}, t - t')$ for $t > t'$, subject to the condition that $G(\mathbf{p}, t - t' < 0) \equiv 0$:

$$\left(\hat{I} i \frac{\partial}{\partial t} - \frac{\hat{I} p^2}{2m} - \bar{\mu}_0 \boldsymbol{\sigma} \cdot \mathbf{B} \right) G(\mathbf{p}, t - t') = \hat{I} \delta(t - t').$$

($\hat{I}$ is the 2×2 unit matrix and $\bar{\mu}_0 = e\hbar/2mc$ is the Bohr magneton.)

1.6 References for Chapter 1

- R.1.1. A. Beiser, "Concepts of Modern Physics," 5th Ed., McGraw-Hill, Inc. (1995). (Elementary introduction to the Schrödinger equation and atomic physics.)
- R.1.2. R.L. Liboff, "Introductory Quantum Mechanics," Holden-Day, Inc. (1980). (Good introduction to quantum mechanics.)
- R.1.3. E. Merzbacher, "Quantum Mechanics," 3rd Ed., John Wiley & Sons, Inc. (1998). (More advanced, fairly comprehensive presentation.)
- R.1.4. P.A.M. Dirac, "Principles of Quantum Mechanics," 3rd Ed., Oxford/Clarendon Press (1949). (The master's voice.)
- R.1.5. J.D. Jackson, "Mathematics for Quantum Mechanics," W.A. Benjamin, Inc. (1962).
- R.1.6. J.J. Sakurai, "Modern Quantum Mechanics," Revised Edition, Editor: San Fu Tuan, Addison-Wesley Publishing Co. (1994).
- R.1.7. R. Shankar, "Principles of Quantum Mechanics," Plenum Press (1980).
- R.1.8. Chen-To Tai, "Dyadic Green's Functions in Electromagnetic Theory," InText Educational Publishers (1971).
- R.1.9. P.M. Morse and H. Feshbach, "Methods of Theoretical Physics," Vol. I, McGraw-Hill Book Co., Inc. (1953).
- R.1.10. L. Page and N.I. Adams, "Electrodynamics," D. van Nostrand Co., Inc. (1940).
- R.1.11. Quoted from the lectures of J. Schwinger on Quantum Mechanics at Harvard University, unpublished (1956).
- R.1.12. J. Schwinger, "The Geometry of Quantum States," Proc. Nat. Academy of Sciences, 46, 257 (1960).
- R.1.13. J. Schwinger, "Quantum Kinematics and Dynamics," W.A. Benjamin, Inc. (1970).
- R.1.14. J. Schwinger, "Quantum Mechanics," Editor: B-G Englert, Springer (2001).

Identical Particles and Second Quantization: Occupation Number Representation

Abstract

Focusing on systems of many identical particles, Chapter 2 introduces appropriate operators to describe their properties in terms of Schwinger's "measurement symbols". The latter are then factorized into "creation" and "annihilation" operators, whose fundamental properties and commutation/anticommutation relations are derived in conjunction with the Pauli exclusion principle. This leads to "second quantization" with the Hamiltonian, number, linear and angular momentum operators expressed in terms of the annihilation and creation operators, as well as the occupation number representation. Finally, the concept of coherent states, as eigenstates of the annihilation operator, having minimum uncertainty, is introduced and discussed in detail.

2.1 Operators for Properties of Identical Particles

In accordance with the quantum mechanical principle of indistinguishability of identical particles, the operators representing their physical properties collectively must be constructed so as to ensure that they cannot be distinguished either kinematically or dynamically.¹ Kinematic identity requires that the particles are described by the same number and kind of dynamical variables, χ_k , such as position $\mathbf{r}_k$ and momentum $\mathbf{p}_k$ operators for each of the particles (indexed by k). Dynamic identity, which assures that the time development of the system does not cause a particular particle to be singled out from the others, requires that the Hamiltonian (which generates time development) must be symmetric with respect to the variables of the constituent particles no matter what perturbations may occur.

Since the constituent particles, which we will now term "subsystems," are therefore perpetually indistinguishable, the collective properties of the whole system must be composed symmetrically from subsystem contributions. For example, considering a property, $F^{(1)}$, of an n -particle system, which is composed of an analogous contribution, $f^{(1)}(\chi_k)$, from each subsystem singly (momentum, angular momentum, kinetic energy, etc.) involving only variables of that subsystem, we have

$$F^{(1)} = \sum_{k=1}^n f^{(1)}(\chi_k) \quad (2.1.1)$$

(e.g., in the case of linear momentum $f^{(1)}(\chi_k) \rightarrow \mathbf{p}_k$ and the total momentum operator is $F^{(1)} \rightarrow \mathbf{P} = \sum_{k=1}^n \mathbf{p}_k$; for angular momentum $f^{(1)}(\chi_k) \rightarrow \mathbf{L}_k$ and $F^{(1)} \rightarrow \mathbf{L} = \sum_{k=1}^n \mathbf{L}_k$ is the total angular momentum operator; and for kinetic energy $f^{(1)}(\chi_k) \rightarrow p_k^2/2m$ and $F^{(1)} \rightarrow KE = \sum_{k=1}^n p_k^2/2m$ is the total kinetic energy operator).

For properties $F^{(2)}$ composed of analogous contributions from each pair of subsystems, such as particle–particle interaction energy, we have

$$F^{(2)} = \sum_{k=1}^n \sum_{\substack{l=1 \\ (k \neq l)}}^n \frac{1}{2!} f^{(2)}(\chi_k, \chi_l). \quad (2.1.2)$$

For example, in the case of the Coulomb interparticle potential, $f^{(2)}(\chi_k, \chi_l) = |\mathbf{r}_k - \mathbf{r}_l|^{-1}$. The exclusion of terms with $k = l$ from $F^{(2)}$ reflects the fact that these terms are of the $f^{(1)}$ type, and the $\frac{1}{2!}$ -factor corrects for double counting in the double sum over k and l . Continuing along these lines, a property $F^{(3)}$ composed of analogous contributions from each triplet of subsystems has the form

$$F^{(3)} = \sum_{k=1}^n \sum_{l=1}^n \sum_{\substack{m=1 \\ (k \neq l \neq m)}}^n \frac{1}{3!} f^{(3)}(\chi_k, \chi_l, \chi_m). \quad (2.1.3)$$

Similar considerations apply to properties $F^{(m)}$ that are composed of analogous contributions involving the joint participation of m subsystems in a group, summed over all such groups of the n -particle system. These n -particle system operator forms ensure that no particle is distinguished from another.

Considering a subsystem k with a complete commuting set of Hermitian operators $A_k = \{A_{1k}, A_{2k}, \dots, A_{lk}\}$ having the single-particle eigenvalue spectrum $\{a'_k\}$ and eigenvectors $|a'_k\rangle$, we may use Eq. (1.4.5) to write

$$f^{(1)}(\chi_k) = \sum_{a'_k, a''_k} \langle a'_k | f^{(1)}(\chi_k) | a''_k \rangle \mathcal{M}(a'_k, a''_k), \quad (2.1.4)$$

where the “measurement symbol,” $\mathcal{M}(a'_k, a''_k)$, is (note that a'_k, a''_k both refer to the spectrum of A_k ; a mixed representation will be discussed below):

$$\mathcal{M}(a'_k, a''_k) = |a'_k\rangle \langle a''_k|. \quad (2.1.5)$$

This corresponds to a measurement that accepts a subsystem in state a''_k and emits it in state a'_k . Because of identity, the spectra of all the subsystems are identical so the index k is irrelevant,

$$a'_k = a', \quad (2.1.6)$$

and it is clear that the matrix element is independent of k ,

$$\langle a'_k | f^{(1)}(\chi_k) | a''_k \rangle \equiv \langle a' | f^{(1)}(\chi) | a'' \rangle, \quad (2.1.7)$$

with the right-hand side being the same for each of the identical subsystems. Thus, from Eqns. (2.1.1) and (2.1.7), we have $\left(\sum_{a'_k, a''_k} \rightarrow \sum_{a', a''}, \text{etc.} \right)$:

$$F^{(1)} = \sum_{a', a''} \langle a' | f^{(1)} | a'' \rangle \mathbf{M}(a', a''), \quad (2.1.8)$$

where

$$\mathbf{M}(a', a'') = \sum_{k=1}^n \mathcal{M}(a'_k, a''_k) \quad (2.1.9)$$

is the *total* measurement symbol, which corresponds to actual observables of the system of identical particles, whereas $\mathcal{M}(a'_k, a''_k)$ can have no direct meaning itself since it refers to a particular subsystem. It should be remarked that, as an operator, $\mathbf{M}(a', a'')$ acts in the product space of the n particles without distinguishing any of them. Clearly, we have the properties

$$\mathbf{M}^+(a', a'') = \mathbf{M}(a'', a'), \quad (2.1.10)$$

and

$$\sum_{a'} \mathbf{M}(a', a') = \sum_{k=1}^n \sum_{a'_k} \mathcal{M}(a'_k, a'_k) = \sum_{k=1}^n \mathbf{I}_k = \mathbf{N} \quad (2.1.11)$$

since

$$\sum_{a'_k} \mathcal{M}(a'_k, a'_k) = \sum_{a'_k} |a'_k\rangle \langle a'_k| = \mathbf{I}_k \quad (2.1.12)$$

is the identity operator for subsystem k , and summation over subsystems then yields the operator $\mathbf{N}$ for the total number of particles of the system, namely n .

Using the orthonormality of the eigenvectors and their adjoints constituting the dyadics $\mathcal{M}(a'_k, a''_k)$, we have (note that $\delta(a', a'')$ is the Kronecker delta for a discrete spectrum and the Dirac delta function for a continuous spectrum):

$$\mathcal{M}(a'_k, a''_k) \mathcal{M}(a'''_k, a^{iv}_k) = \delta(a'', a''') \mathcal{M}(a'_k, a^{iv}_k), \quad (2.1.13)$$

from which we can show that $[A, B] = AB - BA$ is the commutator of A, B)

$$[\mathbf{M}(a', a''), \mathbf{M}(a''', a^{iv})] = \delta(a'', a''') \mathbf{M}(a', a^{iv}) - \delta(a', a^{iv}) \mathbf{M}(a''', a''). \quad (2.1.14)$$

To prove this, we first note that kinematic independence of the subsystems implies that the operators of different subsystems commute with one another,

$$[\mathcal{M}(a'_k, a''_k), \mathcal{M}(a'''_l, a^{iv}_l)] = 0, \quad (k \neq l). \quad (2.1.15)$$

Furthermore (all sums over subsystems are from $1 \rightarrow n$),

$$\begin{aligned} \mathbf{M}(a', a'') \mathbf{M}(a''', a^{iv}) &= \sum_{\substack{k, l \\ (k \neq l)}} \mathcal{M}(a'_k, a''_k) \mathcal{M}(a'''_l, a^{iv}_l) \\ &+ \sum_k \delta(a'', a''') \mathcal{M}(a'_k, a^{iv}_k), \end{aligned} \quad (2.1.16)$$

or, transposing the last term,

$$\mathbf{M}(a', a'') \mathbf{M}(a''', a^{iv}) - \delta(a'', a''') \mathbf{M}(a', a^{iv}) = \sum_{\substack{k, l \\ (k \neq l)}} \mathcal{M}(a'_k, a''_k) \mathcal{M}(a'''_l, a^{iv}_l). \quad (2.1.17)$$

If we now interchange the roles $a', a'' \longleftrightarrow a''', a^{iv}$ and subtract the result from Eq. (2.1.17), the right-hand side vanishes by Eq. (2.1.15), and Eq. (2.1.14) is obtained.

Considering next a property $F^{(2)}$ that is composed of analogous contributions $f^{(2)}(\chi_k, \chi_l)$ from each pair of subsystems ($k \neq l$), a straightforward generalization involving direct product spaces for pairs of particles with basis vectors $|a'_k, a''_l\rangle \equiv |a'_k\rangle |a''_l\rangle$, etc., yields $f^{(2)}(\chi_k, \chi_l)$ in the form

$$f^{(2)}(\chi_k, \chi_l) = \sum_{a'_k, a''_k, a'''_l, a^{iv}_l} \langle a'_k, a'''_l | f^{(2)}(\chi_k, \chi_l) | a''_k, a^{iv}_l \rangle \mathcal{M}(a'_k, a'''_l; a''_k, a^{iv}_l), \quad (2.1.18)$$

where we have defined

$$\mathcal{M}(a'_k, a'''_l; a''_k, a^{iv}_l) \equiv \mathcal{M}(a'_k, a''_k) \mathcal{M}(a'''_l, a^{iv}_l), \quad (2.1.19)$$

which yields an identity when substituted into Eq. (2.1.18). In view of the fact that subsystems/particles are indistinguishable and the matrix elements are independent of particle indices, we may write

$$\begin{aligned} \langle a'_k, a'''_l | f^{(2)}(\chi_k, \chi_l) | a''_k, a^{iv}_l \rangle &= \langle a', a''' | f^{(2)} | a'', a^{iv} \rangle \\ &= \langle a''', a' | f^{(2)} | a^{iv}, a'' \rangle, \end{aligned} \quad (2.1.20)$$

where the last equality reflects the indistinguishability of subsystems interchanged in pairs. Thus, $F^{(2)}$ takes the form

$$F^{(2)} = \sum_{a', a'', a''', a^{iv}} \langle a', a''' | f^{(2)} | a'', a^{iv} \rangle \frac{1}{2!} \sum_{(k \neq l)} \mathcal{M}(a'_k, a''_k) \mathcal{M}(a'''_l, a^{iv}_l). \quad (2.1.21)$$

Eq. (2.1.17) may be used to rewrite $F^{(2)}$ in terms of total measurement symbols, as

$$\begin{aligned} F^{(2)} &= \sum_{a', a'', a''', a^{iv}} \langle a', a''' | f^{(2)} | a'', a^{iv} \rangle \\ &\times \frac{1}{2!} [\mathbf{M}(a', a'') \mathbf{M}(a''', a^{iv}) - \delta(a'', a''') \mathbf{M}(a', a^{iv})]. \end{aligned} \quad (2.1.22)$$

Similarly, $F^{(m)}$ can be written in terms of total measurement symbols alone.

2.2 Second Quantization: Occupation Number Representation

Recalling the interpretation of the single-particle measurement symbol $\mathcal{M}(a'_k, b'_k) = \mathcal{M}(a'_k, 0) \mathcal{M}(0, b'_k)$ as a sequence of operations in which the k^{th} subsystem/particle is annihilated in state $|b'_k\rangle$, followed by the creation/emission of the k^{th} subsystem in state $|a'_k\rangle$ with the original amplitude of the state $|b'_k\rangle$, it is clear that the total measurement symbol,

$$\mathbf{M}(a', b') = \sum_{k=1}^n \mathcal{M}(a'_k, b'_k), \quad (2.2.1)$$

has a similar interpretation. It operates on a system by removing/annihilating a subsystem in *mode* b' , and creates a subsystem in *mode* a' , without distinguishing which particular subsystem/particle is annihilated/created, since the contributions of all subsystems to $\mathbf{M}(a', b')$ in Eq. (2.2.1) are equally weighted and symmetrical. Moreover, the sum $\sum_{k=1}^n$ in Eq. (2.2.1) signifies the “either/or” logic of addition, so that just one subsystem undergoes the sequence of annihilation and creation operations, anonymously.

The interpretive scheme described previously can be given mathematical expression by introducing “second quantized” field operators $\psi^+(a')$, $\psi(b')$, such that $\mathbf{M}(a', b')$ is factored using the two operators as

$$\mathbf{M}(a', b') = \psi^+(a') \psi(b'), \quad (2.2.2)$$

where $\psi(b')$ is defined to annihilate a subsystem in *mode* b' and $\psi^+(a')$ is defined to create a subsystem in *mode* a' . This decomposition of $\mathbf{M}(a', b')$ is done in analogy to Eq. (1.4.8), with interpretations of $\psi(b')$ and $\psi^+(a')$ fully analogous to the interpretations of $\mathcal{M}(0, b')$ and $\mathcal{M}(a', 0) = \mathcal{M}^+(0, a')$, respectively, except that in the present context the indistinguishability of particles means that it is not possible to determine which particular

subsystems are annihilated/created, since all of them are represented with equal weight in $\mathbf{M}(a', b')$. The transformation properties of $\mathbf{M}(a', b')$ under a change of representation are readily obtained as

$$\mathbf{M}(c', d') = \sum_{a', b'} \langle a' | c' \rangle \mathbf{M}(a', b') \langle d' | b' \rangle, \quad (2.2.3)$$

and they lead at once to the corresponding transformation properties for $\psi(a')$, $\psi^+(b')$, as

$$\begin{aligned} \psi(a') &= \sum_{b'} \langle a' | b' \rangle \psi(b') \\ \psi^+(b') &= \sum_{a'} \psi^+(a') \langle a' | b' \rangle, \end{aligned} \quad (2.2.4)$$

since $\langle a' | b' \rangle = \langle b' | a' \rangle^*$. Moreover, since $F^{(1)}$ may be written in a mixed representation as

$$F^{(1)} = \sum_{a', b'} \langle a' | f^{(1)} | b' \rangle \mathbf{M}(a', b'), \quad (2.2.5)$$

we have

$$F^{(1)} = \sum_{a', b'} \psi^+(a') \langle a' | f^{(1)} | b' \rangle \psi(b'). \quad (2.2.6)$$

It is necessary to recognize that the mathematical implementation of this interpretive scheme requires the introduction of a Fock or a “number” space,² in which particle numbers may change with the annihilation or creation of subsystems. The description of a state, correspondingly, is given in terms of the occupation numbers of given subsystem modes and associated linear superpositions. For example, instead of describing a state of non-interacting particles by symmetrized/antisymmetrized products of the wave functions of n particles (Eq. (1.1.42)), the number space description is lodged merely in terms of the occupation numbers of the constituent subsystem modes.

The realization of the annihilation and creation properties of $\psi(a')$, $\psi^+(a')$ in terms of number space operations may be discussed by starting with Eq. (2.1.11),

$$\sum_{a'} \mathbf{M}(a', a') = \mathbf{N} = \sum_{a'} \psi^+(a') \psi(a'), \quad (2.2.7)$$

where $\mathbf{N}$ is the operator whose eigenvalues are the total (integer) number of particles, n , in the system, with eigenvector $|n\rangle$, $\mathbf{N}|n\rangle = n|n\rangle$. Moreover, the operator for the number of particles having eigenvalue a' of the $\mathbf{A}$ spectrum is $\psi^+(a')\psi(a')$. In position representation (and taking account of internal coordinates ξ , like spin),

$$\mathbf{N} = \int d^{(3)}\mathbf{x} \sum_{\xi} \psi^+(\mathbf{x}, \xi) \psi(\mathbf{x}, \xi). \quad (2.2.8)$$

Clearly, the operator for the particle density with spin ξ is just the integrand,

$$\rho(\mathbf{x}, \xi) = \psi^\dagger(\mathbf{x}, \xi) \psi(\mathbf{x}, \xi). \quad (2.2.9)$$

Considering the annihilation properties of $\psi(a')$, the state $\psi(a')|n\rangle$ must have one less particle than does $|n\rangle$, so its number eigenvalue is reduced by one:

$$\mathbf{N}\psi(a')|n\rangle = (n-1)\psi(a')|n\rangle \quad (2.2.10)$$

(this state, $\psi(a')|n\rangle$, is *not* normalized to unity). Noting that $\mathbf{N}|n\rangle = n|n\rangle$, this relation may be alternatively written as

$$\mathbf{N}\psi(a')|n\rangle = \psi(a')(\mathbf{N}-\mathbf{I})|n\rangle. \quad (2.2.11)$$

Since this is true for every value of n , we have

$$\mathbf{N}\psi(a') = \psi(a')(\mathbf{N}-\mathbf{I}), \quad (2.2.12)$$

and, similarly, since the creation operator $\psi^\dagger(a')$ increases by one the number of particles of the state $|n\rangle$ upon which it acts, we also have

$$\mathbf{N}\psi^\dagger(a') = \psi^\dagger(a')(\mathbf{N}+\mathbf{I}). \quad (2.2.13)$$

Eqns. (2.2.12) and (2.2.13) may be written as

$$\begin{aligned} [\psi(a'), \mathbf{N}] &= \psi(a'), \\ [\psi^\dagger(a'), \mathbf{N}] &= -\psi^\dagger(a'). \end{aligned} \quad (2.2.14)$$

Since $\mathbf{N}=\mathbf{N}^\dagger$ is Hermitian, the two equations in Eq. (2.2.14) are just Hermitian adjoints of each other. These considerations are easily generalized to arbitrary operator functions of $\mathbf{N}$, $f(\mathbf{N})$:

$$\begin{aligned} f(\mathbf{N})\psi(a') &= \psi(a')f(\mathbf{N}-\mathbf{I}), \\ f(\mathbf{N})\psi^\dagger(a') &= \psi^\dagger(a')f(\mathbf{N}+\mathbf{I}). \end{aligned} \quad (2.2.15)$$

An important special case is the unitary operator $e^{i\phi\mathbf{N}}$ (ϕ is a real phase):

$$e^{-i\phi\mathbf{N}}\psi(a') = \psi(a')e^{-i\phi(\mathbf{N}-\mathbf{I})}, \quad (2.2.16)$$

whence

$$e^{-i\phi\mathbf{N}}\psi(a')e^{i\phi\mathbf{N}} = e^{i\phi}\psi(a'), \quad (2.2.17)$$

and taking the adjoint,

$$e^{-i\phi N} \psi^+(a') e^{i\phi N} = e^{-i\phi} \psi^+(a'). \quad (2.2.18)$$

If we consider the addition of two particles to the system, one in state a' and one in state a'' , we have

$$\psi^+(a') \psi^+(a'') |n\rangle = |n + 1_{a'} + 1_{a''}\rangle \text{ (unnormalized)} \quad (2.2.19)$$

(normalization will be discussed below). Adding the particles in the reverse order,

$$\psi^+(a'') \psi^+(a') |n\rangle = |n + 1_{a''} + 1_{a'}\rangle \text{ (unnormalized)} \quad (2.2.20)$$

must have the same physical result, so the states on the right-hand sides of the Eqns. (2.2.19) and (2.2.20) can differ only by a phase factor, $e^{i\theta}$. Correspondingly, the left-hand sides of these equations are related by

$$\psi^+(a') \psi^+(a'') = e^{i\theta} \psi^+(a'') \psi^+(a'). \quad (2.2.21)$$

(Note that any dependence of the phase factor on a', a'' is ruled out by the requirement that the result be consistent with the known transformation properties of ψ^+, ψ in Eq. (2.2.4).) Clearly, a second application of Eq. (2.2.21) to bring the order of $\psi^+(a'') \psi^+(a')$ on the right back to $\psi^+(a') \psi^+(a'')$ invokes a second phase factor, so

$$e^{2i\theta} = 1 \ ; \ e^{i\theta} = \pm 1 \quad (2.2.22)$$

is required for consistency. Therefore, there are two types of systems:

(a) First kind, $\pm \rightarrow +$,

$$[\psi(a'), \psi(a'')] = [\psi^+(a'), \psi^+(a'')] = 0, \quad (2.2.23)$$

where $[A, B] \equiv (AB - BA)$ is the commutator of A, B .

(b) Second kind, $\pm \rightarrow -$,

$$\{\psi(a'), \psi(a'')\} = \{\psi^+(a'), \psi^+(a'')\} = 0, \quad (2.2.24)$$

where $\{A, B\} \equiv (AB + BA)$ is the anticommutator of A, B .

Furthermore, considering Eqns. (2.2.14), we have

$$\left[\psi(a'), \sum_{a''} \psi^+(a'') \psi(a'') \right] = \psi(a'), \quad (2.2.25)$$