

Springer Series on

ATOMIC, OPTICAL, AND PLASMA PHYSICS 47

Springer Series on

ATOMIC, OPTICAL, AND PLASMA PHYSICS

The Springer Series on Atomic, Optical, and Plasma Physics covers in a comprehensive manner theory and experiment in the entire field of atoms and molecules and their interaction with electromagnetic radiation. Books in the series provide a rich source of new ideas and techniques with wide applications in fields such as chemistry, materials science, astrophysics, surface science, plasma technology, advanced optics, aeronomy, and engineering. Laser physics is a particular connecting theme that has provided much of the continuing impetus for new developments in the field. The purpose of the series is to cover the gap between standard undergraduate textbooks and the research literature with emphasis on the fundamental ideas, methods, techniques, and results in the field.

- 36 **Atom Tunneling Phenomena in Physics, Chemistry and Biology**
Editor: T. Miyazaki
- 37 **Charged Particle Traps**
Physics and Techniques of Charged Particle Field Confinement
By V.N. Gheorghe, F.G. Major, G. Werth
- 38 **Plasma Physics and Controlled Nuclear Fusion**
By K. Miyamoto
- 39 **Plasma-Material Interaction in Controlled Fusion**
By D. Naujoks
- 40 **Relativistic Quantum Theory of Atoms and Molecules**
Theory and Computation
By I.P. Grant
- 41 **Turbulent Particle-Laden Gas Flows**
By A.Y. Varaksin
- 42 **Phase Transitions of Simple Systems**
By B.M. Smirnov and S.R. Berry
- 43 **Collisions of Charged Particles with Molecules**
By Y. Itikawa
- 44 **Collisions of Charged Particles with Molecules**
Editors: T. Fujimoto and A. Iwamae
- 45 **Emergent Nonlinear Phenomena in Bose-Einstein Condensates**
Theory and Experiment
Editors: P.G. Kevrekidis, D.J. Frantzeskakis, and R. Carretero-González
- 46 **Angle and Spin Resolved Auger Emission**
Theory and Applications to Atoms and Molecules
By: B. Lohmann
- 47 **Semiclassical Dynamics and Relaxation**
By: D.S.F. Crothers

Vols. 10-35 of the former Springer Series on Atoms and Plasmas are listed at the end of the book

D.S.F. Crothers

Semiclassical Dynamics and Relaxation

With 56 Figures

 Springer

D.S.F. Crothers
Department of Applied Mathematics
and Theoretical Physics
Queen's University of Belfast, UK
University Road
Belfast BT7 1NN
E-mail: d.crothers@qub.ac.uk

ISBN: 978-0-387-74312-7

e-ISBN: 978-0-387-74313-4

Library of Congress Control Number: 2007940870

© 2008 Springer Science+Business Media, LLC

All rights reserved. This work may not be translated or copied in whole or in part without the written permission of the publisher (Springer Science+Business Media, LLC, 233 Spring Street, New York, NY 10013, USA), except for brief excerpts in connection with reviews or scholarly analysis. Use in connection with any form of information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed is forbidden.

The use in this publication of trade names, trademarks, service marks and similar terms, even if they are not identified as such, is not to be taken as an expression of opinion as to whether or not they are subject to proprietary rights.

Printed on acid-free paper.

9 8 7 6 5 4 3 2 1

springer.com

I dedicate this book to the memory of my mentor and supervisor, the late Professor Sir David Bates FRS. I gratefully acknowledge my teachers: at Rainey Endowed School: the late Mr Thomas Fazackerley (applied mathematics), the late Dr Arthur Gwilliam (pure mathematics), and the late Mr James McAteer (physics), at Balliol College Oxford: the late Professor Jacobus Stephanus de Wet (applied mathematics) and the late Dr Kenneth Gravett (pure mathematics), and at Queen's University Belfast my other supervisor Professor Ron McCarroll.

I warmly acknowledge fruitful collaboration with Professors Anders Barany, Alex Devdariani, Bill Coffey, Yura Kalmykov, Kanika Roy, and Vladimir Gaiduk. I also thank my 32 PhD students for their inspiring hard work and collaboration and my wife Eithne for her loving care. Of my 32 PhD students I particularly thank my colleagues Dr Jim McCann and Dr Francesca O'Rourke, each of whom I have collaborated with over the years. I also thank my former postdocs: Dr Narayan Deb, Dr Geoffrey Brown, Dr P.J. Cregg, Dr Lawrence Geoghegan, Dr Elaine Kennedy, Dr Arlene Loughan, Dr Pierre-Michel Dejardin, Dr Elena Bichoutskaia, and Dr Sergei Titov. I thank Miss (soon to be Dr) Carla McGrath for her wonderfully precise typing of this book in Springer-Latex. Last but not least, I profoundly thank Carla and Elizabeth (Dr O'Sullivan) for their industrious application of Springer corrections to the final version.

Preface

The eclectic choice of topics in the book reflects the author's research interests over forty four years, before which he was War Memorial Open Scholar in Mathematics at Balliol College Oxford (1960–1963). Accordingly Chapter 1 covers some good oldfashioned applied mathematics of relevance to Chapters 2–4 concerning atomic and molecular physics in the gaseous phase (single collisions at low pressures) and to Chapter 5 concerning condensed-matter physics in the liquid and solid phases (dielectrics and ferromagnetics). The five chapters are based on a set of five special lectures given to postgraduate PhD students in the Centre for Atomic, Molecular and Optical Physics, in the School of Mathematics and Physics, Queen's University Belfast, in May and June 2003. The author was appointed to a Personal Chair in Theoretical Physics at Queen's University Belfast (1985), and elected as Member of the Royal Irish Academy (1991), Fellowship of the American Physical Society (1994), Honorary Professor of Physics at St Petersburg State University (2003) and Honorary Fellow of Trinity College Dublin (2006).

A good introduction to Chapters 3 and 4 is given by Chapter 52 (Continuum Distorted Waves and Wannier Methods by D.S.F. Crothers et al) of the Springer Handbook of Atomic, Molecular and Optical Physics (ed G.W.F. Drake), 2006.

Belfast,
Northern Ireland

Derrick Crothers
April 2007

Contents

1	Mathematics for the Semiclassicist	1
1.1	Single-Valued Analytic Functions	1
1.2	Method of Steepest Descent and Asymptotic Methods	2
1.2.1	Stationary-Phase Version	3
1.3	Generalized Variation and Perturbation Theories	4
1.4	Hypergeometric Series	6
1.5	Contour Integral Transforms	11
1.6	Combinatorics	14
1.6.1	Proof via Sister Celine’s Technique	15
1.7	Generalized Hypergeometric Functions	16
1.8	Fourier and Laplace Transforms	19
1.8.1	Critical Fourier Transform Relation	19
1.8.2	Critical Laplace Transform Relation	20
2	Semiclassical Phase Integrals	21
2.1	Approximation	21
2.1.1	JWKB Approximation	21
2.1.2	Gans–Jeffreys Asymptotic Connection Formula	24
2.2	Phase Integrals	25
2.2.1	Stokes Phenomenon: One Transition Point	25
2.2.2	Application of JWKB to Coupled Wave Equations	29
2.3	Two and Four Transition Points: Crossing and Noncrossing	44
2.3.1	Introduction	44
2.3.2	Exact Resumming of Asymptotic Relations for Parabolic Cylinder Functions of Large Order and Argument	45
2.3.3	The Crossing Parabolic Model	58
2.3.4	Connection to Barany–Crothers Phase-Integral Nikitin–Model Analysis	61
2.3.5	Connections to Nakamura and Zhu Phase-Integral Analysis	62
2.3.6	Connections to the Fromans–Lundborg Phase-Integral Analysis	64

2.3.7	Conclusions	65
2.3.8	Curve Crossing Reflection Probabilities in One Dimension	66
2.4	Addition of a Simple Pole	71
2.4.1	Introduction	71
2.4.2	The Semiclassical Scattering Matrix	74
2.4.3	Phase-Integral Treatment	75
2.4.4	Comparison Equation	80
2.4.5	General Phase-Integral Abstraction	83
2.4.6	Discussion	83
2.5	Other Generalizations	85
2.5.1	Four Close Curve-Crossing Transition Points	85
2.5.2	Circuit-Dependent Adiabatic Phase Factors from Phase Integral Theory	88
3	Semiclassical Method for Hyperspherical Coordinate Systems	93
3.1	Wannier's Classical Treatment of Electron Correlation	93
3.2	Differential and Integrated Wannier Cross Sections	98
3.2.1	Conclusions	115
3.3	Doubly Excited States and Their Lifetimes	116
3.3.1	Results	123
3.3.2	Doubly Excited States of He	125
3.4	Divergent Exponents	128
3.4.1	Wannier's Theory	129
3.4.2	The Semiclassical JWKB Approximation	130
3.4.3	Semiclassical Theory when the Exponent Diverges	131
3.4.4	Results, Discussion, and Conclusions	137
4	Ion-Atom Collisions	139
4.1	The Semiclassical Impact Parameter Treatment	139
4.2	Traveling Atomic and Molecular Orbitals	144
4.2.1	Traveling Molecular H_2^+ Orbitals	145
4.2.2	Traveling Molecular HeH^{2+} Orbitals	155
4.2.3	Traveling Atomic Orbitals	171
4.3	Continuum Distorted Waves and Their Generalizations	172
4.3.1	Introduction	172
4.3.2	Charge Transfer	173
4.3.3	Ionization	182
4.3.4	Fully differential cross sections for ionization	197
4.3.5	Generalized Continuum Distorted Waves	210
4.3.6	Double Ionization	215
4.4	Relativistic CDW	219
4.4.1	Antihydrogen Production	231
4.5	Semiclassical Acausality	234
4.5.1	Introduction	234
4.5.2	Generalized Impact-Parameter Treatment	236

4.5.3	Perturbation Theory	238
4.5.4	Discussion and Conclusions	240
5	Diffusion in Liquids and Solids	243
5.1	Single-Domain Ferromagnetic Particles	243
5.2	The Fokker–Planck and Langevin Equations	267
5.2.1	Drift and Diffusion Coefficients	273
5.3	Dielectric Relaxation, Anomalous Diffusion, Fractals, and After Effects	284
5.3.1	Numerical Calculation and Physical Understanding	289
5.4	Nonlinear Response of Permanent Dipoles and After Effects	292
5.4.1	Complex Susceptibility for the Debye and Debye–Fröhlich Models of Relaxation	294
5.4.2	Linear Dielectric Response	297
5.4.3	Dynamic Kerr Effect	299
5.4.4	Nonlinear Dielectric Relaxation	300
5.4.5	Approximate Analytical Formula for the Dynamic Kerr Effect for a Pure Cosinusoid	301
A	Continued Fraction Solutions of Eq. (5.301)	305
B	Mittag–Leffler Functions	309
B.0.1	Properties of Mittag–Leffler Functions	309
B.0.2	Asymptotics of Mittag–Leffler functions	309
B.1	Check on Norm of $x^2(\tau)$	311
C	Nonlinear Response to Alternating Fields	313
	References	321
	Index	337