

## Computational Methods for Electromagnetic Phenomena

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- Absorbing and UPML boundary conditions
- High-order hierarchical Nédélec edge elements
- High-order discontinuous Galerkin (DG) and Yee scheme time-domain methods
- Finite element and plane wave frequency-domain methods for periodic structures
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- NEGF (non-equilibrium Green’s function) and Wigner kinetic methods for quantum transport
- High-order WENO, Godunov and central schemes for hydrodynamic transport
- Vlasov–Fokker–Planck, PIC, and constrained MHD transport in plasmas

**WEI CAI** has been a full Professor at the University of North Carolina since 1999. He has also taught and conducted research at Peking University, Fudan University, Shanghai Jiaotong University, and the University of California, Santa Barbara. He has published over 90 refereed journal articles, and was awarded the prestigious Feng Kang prize in scientific computing in 2005.

*“A well-written book which will be of use to a broad range of students and researchers in applied mathematics, applied physics and engineering. It provides a clear presentation of many topics in computational electromagnetics and illustrates their importance in a distinctive and diverse set of applications.”*

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*“... This is a truly unique book that covers a variety of computational methods for several important physical (electromagnetics) problems in a rigorous manner with a great depth. It will benefit not only computational mathematicians, but also physicists and electrical engineers interested in numerical analysis of electrostatic, electrodynamic, and electron transport problems. The breadth (both in terms of physics and numerical analysis) and depth are very impressive. I like, in particular, the way the book is organized: A physical problem is described clearly first and then followed by the presentation of relevant state-of-the-art computational methods...”*

— Jian-Ming Jin, Y. T. Lo Chair Professor in Electrical and Computer Engineering,  
University of Illinois at Urbana-Champaign

*“This book is a great and unique contribution to computational modeling of electromagnetic problems across many fields, covering in depth all interesting multi-scale phenomena, from electrostatics in biomolecules, to EM scattering, to electron transport in plasmas, and quantum electron transport in semiconductors. It includes both atomistic descriptions and continuum based formulations with emphasis on long-range interactions and high-order algorithms, respectively. The book is divided into three main parts and includes both established but also new algorithms on every topic addressed, e.g. fast multipole expansions, boundary integral equations, high-order finite elements, discontinuous Galerkin and WENO methods. Both the organization of the material and the exposition of physical and algorithmic concepts is superb and make the book accessible to researchers and students in every discipline.”*

— George Karniadakis, Professor of Applied Mathematics, Brown University

*“This is an impressive ... excellent book for those who want to study and understand the relationship between mathematical methods and the many different physical problems they can model and solve.”*

— Weng Cho Chew, First Y. T. Lo Endowed Chair Professor in Electrical and  
Computer Engineering, University of Illinois at Urbana-Champaign

# Computational Methods for Electromagnetic Phenomena

Electrostatics in Solvation, Scattering,  
and Electron Transport

WEI CAI

University of North Carolina



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To my wife, Xiaoyan,

and

my children, Angela and Richard

## Contents

<i>Foreword</i>	<i>page</i> xiv
<i>Preface</i>	xv
<b>Part I Electrostatics in solvation</b>	<b>1</b>
<b>1 Dielectric constant and fluctuation formulae for molecular dynamics</b>	<b>3</b>
1.1 Electrostatics of charges and dipoles	3
1.2 Polarization $\mathbf{P}$ and displacement flux $\mathbf{D}$	5
1.2.1 Bound charges induced by polarization	6
1.2.2 Electric field $\mathbf{E}_{\text{pol}}(\mathbf{r})$ of a polarization density $\mathbf{P}(\mathbf{r})$	7
1.2.3 Singular integral expressions of $\mathbf{E}_{\text{pol}}(\mathbf{r})$ inside dielectrics	9
1.3 Clausius–Mossotti and Onsager formulae for dielectric constant	9
1.3.1 Clausius–Mossotti formula for non-polar dielectrics	9
1.3.2 Onsager dielectric theory for dipolar liquids	11
1.4 Statistical molecular theory and dielectric fluctuation formulae	16
1.4.1 Statistical methods for polarization density change $\Delta\mathbf{P}$	18
1.4.2 Classical electrostatics for polarization density change $\Delta\mathbf{P}$	20
1.4.3 Fluctuation formulae for dielectric constant $\epsilon$	21
1.5 Appendices	23
1.5.1 Appendix A: Average field of a charge in a dielectric sphere	23
1.5.2 Appendix B: Electric field due to a uniformly polarized sphere	24
1.6 Summary	25
<b>2 Poisson–Boltzmann electrostatics and analytical approximations</b>	<b>26</b>
2.1 Poisson–Boltzmann (PB) model for electrostatic solvation	26
2.1.1 Debye–Hückel Poisson–Boltzmann theory	27
2.1.2 Helmholtz double layer and ion size effect	30
2.1.3 Electrostatic solvation energy	34
2.2 Generalized Born (GB) approximations of solvation energy	36
2.2.1 Still’s generalized Born formulism	37
2.2.2 Integral expression for Born radii	37
2.2.3 FFT-based algorithm for the Born radii	39
2.3 Method of images for reaction fields	44

2.3.1	Methods of images for simple geometries	45
2.3.2	Image methods for dielectric spheres	47
2.3.3	Image methods for dielectric spheres in ionic solvent	53
2.3.4	Image methods for multi-layered media	55
2.4	Summary	59
<b>3</b>	<b>Numerical methods for Poisson–Boltzmann equations</b>	<b>60</b>
3.1	Boundary element methods (BEMs)	60
3.1.1	Cauchy principal value (CPV) and Hadamard finite part (p.f.)	61
3.1.2	Surface integral equations for the PB equations	65
3.1.3	Computations of CPV and Hadamard p.f. and collocation BEMs	71
3.2	Finite element methods (FEMs)	82
3.3	Immersed interface methods (IIMs)	85
3.4	Summary	88
<b>4</b>	<b>Fast algorithms for long-range interactions</b>	<b>89</b>
4.1	Ewald sums for charges and dipoles	89
4.2	Particle-mesh Ewald (PME) methods	96
4.3	Fast multipole methods for $N$ -particle electrostatic interactions	98
4.3.1	Multipole expansions	98
4.3.2	A recursion for the local expansions ( $0 \rightarrow L$ -level)	102
4.3.3	A recursion for the multipole expansions ( $L \rightarrow 0$ -level)	104
4.3.4	A pseudo-code for FMM	104
4.3.5	Conversion operators for electrostatic FMM in $\mathbb{R}^3$	105
4.4	Helmholtz FMM of wideband of frequencies for $N$ -current source interactions	107
4.5	Reaction field hybrid model for electrostatics	110
4.6	Summary	116
<b>Part II</b>	<b>Electromagnetic scattering</b>	<b>117</b>
<b>5</b>	<b>Maxwell equations, potentials, and physical/artificial boundary conditions</b>	<b>119</b>
5.1	Time-dependent Maxwell equations	119
5.1.1	Magnetization $\mathbf{M}$ and magnetic field $\mathbf{H}$	120
5.2	Vector and scalar potentials	122
5.2.1	Electric and magnetic potentials for time-harmonic fields	123
5.3	Physical boundary conditions for $\mathbf{E}$ and $\mathbf{H}$	125
5.3.1	Interface conditions between dielectric media	125
5.3.2	Leontovich impedance boundary conditions for conductors	127
5.3.3	Sommerfeld and Silver–Müller radiation conditions	129
5.4	Absorbing boundary conditions for $\mathbf{E}$ and $\mathbf{H}$	132

	Contents	ix
	5.4.1 One-way wave Engquist–Majda boundary conditions	132
	5.4.2 High-order local non-reflecting Bayliss–Turkel conditions	134
	5.4.3 Uniaxial perfectly matched layer (UPML)	138
	5.5 Summary	144
6	<b>Dyadic Green’s functions in layered media</b>	145
6.1	Singular charge and current sources	145
6.1.1	Singular charge sources	145
6.1.2	Singular Hertz dipole current sources	147
6.2	Dyadic Green’s functions $\overline{\mathbf{G}}_E(\mathbf{r} \mathbf{r}')$ and $\overline{\mathbf{G}}_H(\mathbf{r} \mathbf{r}')$	148
6.2.1	Dyadic Green’s functions for homogeneous media	149
6.2.2	Dyadic Green’s functions for layered media	150
6.2.3	Hankel transform for radially symmetric functions	150
6.2.4	Transverse versus longitudinal field components	152
6.2.5	Longitudinal components of Green’s functions	153
6.3	Dyadic Green’s functions for vector potentials $\overline{\mathbf{G}}_A(\mathbf{r} \mathbf{r}')$	157
6.3.1	Sommerfeld potentials	158
6.3.2	Transverse potentials	160
6.4	Fast computation of dyadic Green’s functions	160
6.5	Appendix: Explicit formulae	165
6.5.1	Formulae for $\tilde{G}_1$ , $\tilde{G}_2$ , and $\tilde{G}_3$ , etc.	165
6.5.2	Closed-form formulae for $\tilde{\psi}(k_\rho)$	167
6.6	Summary	169
7	<b>High-order methods for surface electromagnetic integral equations</b>	170
7.1	Electric and magnetic field surface integral equations in layered media	170
7.1.1	Integral representations	170
7.1.2	Singular and hyper-singular surface integral equations	175
7.2	Resonance and combined integral equations	182
7.3	Nyström collocation methods for Maxwell equations	185
7.3.1	Surface differential operators	185
7.3.2	Locally corrected Nyström method for hyper-singular EFIE	186
7.3.3	Nyström method for mixed potential EFIE	190
7.4	Galerkin methods and high-order RWG current basis	191
7.4.1	Galerkin method using vector–scalar potentials	191
7.4.2	Functional space for surface current $\mathbf{J}(\mathbf{r})$	192
7.4.3	Basis functions over triangular–triangular patches	194
7.4.4	Basis functions over triangular–quadrilateral patches	198
7.5	Summary	203
8	<b>High-order hierarchical Nédélec edge elements</b>	205
8.1	Nédélec edge elements in $H(\text{curl})$	205
8.1.1	Finite element method for $\mathbf{E}$ or $\mathbf{H}$ wave equations	206



8.1.2	Reference elements and Piola transformations	208
8.1.3	Nédélec finite element basis in $H(\text{curl})$	209
8.2	Hierarchical Nédélec basis functions	217
8.2.1	Construction on 2-D quadrilaterals	218
8.2.2	Construction on 2-D triangles	219
8.2.3	Construction on 3-D cubes	222
8.2.4	Construction on 3-D tetrahedra	223
8.3	Summary	227
<b>9</b>	<b>Time-domain methods – discontinuous Galerkin method and Yee scheme</b>	<b>228</b>
9.1	Weak formulation of Maxwell equations	228
9.2	Discontinuous Galerkin (DG) discretization	229
9.3	Numerical flux $\mathbf{h}(\mathbf{u}^-, \mathbf{u}^+)$	230
9.4	Orthonormal hierarchical basis for DG methods	234
9.4.1	Orthonormal hierarchical basis on quadrilaterals or hexahedra	234
9.4.2	Orthonormal hierarchical basis on triangles or tetrahedra	234
9.5	Explicit formulae of basis functions	236
9.6	Computation of whispering gallery modes (WGMs) with DG methods	238
9.6.1	WGMs in dielectric cylinders	238
9.6.2	Optical energy transfer in coupled micro-cylinders	239
9.7	Finite difference Yee scheme	242
9.8	Summary	245
<b>10</b>	<b>Scattering in periodic structures and surface plasmons</b>	<b>247</b>
10.1	Bloch theory and band gap for periodic structures	247
10.1.1	Bloch theory for 1-D periodic Helmholtz equations	248
10.1.2	Bloch wave expansions	250
10.1.3	Band gaps of photonic structures	250
10.1.4	Plane wave method for band gap calculations	252
10.1.5	Rayleigh–Bloch waves and band gaps by transmission spectra	253
10.2	Finite element methods for periodic structures	257
10.2.1	Nédélec edge element for eigen-mode problems	257
10.2.2	Time-domain finite element methods for periodic array antennas	261
10.3	Physics of surface plasmon waves	265
10.3.1	Propagating plasmons on planar surfaces	265
10.3.2	Localized surface plasmons	268
10.4	Volume integral equation (VIE) for Maxwell equations	270
10.5	Extraordinary optical transmission (EOT) in thin metallic films	273
10.6	Discontinuous Galerkin method for resonant plasmon couplings	274

10.7	Appendix: Auxiliary differential equation (ADE) DG methods for dispersive Maxwell equations	276
10.7.1	Debye material	277
10.7.2	Drude material	282
10.8	Summary	283
<b>11</b>	<b>Schrödinger equations for waveguides and quantum dots</b>	<b>284</b>
11.1	Generalized DG (GDG) methods for Schrödinger equations	284
11.1.1	One-dimensional Schrödinger equations	284
11.1.2	Two-dimensional Schrödinger equations	287
11.2	GDG beam propagation methods (BPMs) for optical waveguides	289
11.2.1	Guided modes in optical waveguides	289
11.2.2	Discontinuities in envelopes of guided modes	294
11.2.3	GDG-BPM for electric fields	296
11.2.4	GDG-BPM for magnetic fields	299
11.2.5	Propagation of $HE_{11}$ modes	301
11.3	Volume integral equations for quantum dots	302
11.3.1	One-particle Schrödinger equation for electrons	302
11.3.2	VIE for electrons in quantum dots	304
11.3.3	Derivation of the VIE for quantum dots embedded in layered media	306
11.4	Summary	309
<b>Part III</b>	<b>Electron transport</b>	<b>311</b>
<b>12</b>	<b>Quantum electron transport in semiconductors</b>	<b>313</b>
12.1	Ensemble theory for quantum systems	313
12.1.1	Thermal equilibrium of a quantum system	313
12.1.2	Microcanonical ensembles	315
12.1.3	Canonical ensembles	316
12.1.4	Grand canonical ensembles	319
12.1.5	Bose–Einstein and Fermi–Dirac distributions	320
12.2	Density operator $\hat{\rho}$ for quantum systems	324
12.2.1	One-particle density matrix $\rho(x, x')$	328
12.3	Wigner transport equations and Wigner–Moyal expansions	329
12.4	Quantum wave transmission and Landauer current formula	335
12.4.1	Transmission coefficient $T(E)$	335
12.4.2	Current formula through barriers via $T(E)$	337
12.5	Non-equilibrium Green’s function (NEGF) and transport current	341
12.5.1	Quantum devices with one contact	342
12.5.2	Quantum devices with two contacts	346
12.5.3	Green’s function and transport current formula	348
12.6	Summary	348

<b>13</b>	<b>Non-equilibrium Green's function (NEGF) methods for transport</b>	<b>349</b>
13.1	NEGFs for 1-D devices	349
13.1.1	1-D device boundary conditions for Green's functions	349
13.1.2	Finite difference methods for 1-D device NEGFs	351
13.1.3	Finite element methods for 1-D device NEGFs	353
13.2	NEGFs for 2-D devices	354
13.2.1	2-D device boundary conditions for Green's functions	354
13.2.2	Finite difference methods for 2-D device NEGFs	357
13.2.3	Finite element methods for 2-D device NEGFs	359
13.3	NEGF simulation of a <b>29</b> nm double gate MOSFET	361
13.4	Derivation of Green's function in 2-D strip-shaped contacts	363
13.5	Summary	364
<b>14</b>	<b>Numerical methods for Wigner quantum transport</b>	<b>365</b>
14.1	Wigner equations for quantum transport	365
14.1.1	Truncation of phase spaces and charge conservation	365
14.1.2	Frensley inflow boundary conditions	367
14.2	Adaptive spectral element method (SEM)	367
14.2.1	Cell averages in $k$ -space	368
14.2.2	Chebyshev collocation methods in $x$ -space	372
14.2.3	Time discretization	372
14.2.4	Adaptive meshes for Wigner distributions	374
14.3	Upwinding finite difference scheme	375
14.3.1	Selections of $L_{\text{coh}}$ , $N_{\text{coh}}$ , $L_k$ , and $N_k$	375
14.3.2	Self-consistent algorithm through the Poisson equation	376
14.3.3	Currents in RTD by NEGF and Wigner equations	377
14.4	Calculation of oscillatory integrals $O_n(z)$	378
14.5	Summary	379
<b>15</b>	<b>Hydrodynamic electron transport and finite difference methods</b>	<b>380</b>
15.1	Semi-classical and hydrodynamic models	380
15.1.1	Semi-classical Boltzmann equations	380
15.1.2	Hydrodynamic equations	381
15.2	High-resolution finite difference methods of Godunov type	388
15.3	Weighted essentially non-oscillatory (WENO) finite difference methods	392
15.4	Central differencing schemes with staggered grids	396
15.5	Summary	400
<b>16</b>	<b>Transport models in plasma media and numerical methods</b>	<b>402</b>
16.1	Kinetic and macroscopic magneto-hydrodynamic (MHD) theories	402
16.1.1	Vlasov–Fokker–Planck equations	402
16.1.2	MHD equations for plasma as a conducting fluid	404
16.2	Vlasov–Fokker–Planck (VFP) schemes	410

	Contents	xiii
16.3	Particle-in-cell (PIC) schemes	413
16.4	$\nabla \cdot \mathbf{B} = 0$ constrained transport methods for MHD equations	414
16.5	Summary	418
	<i>References</i>	419
	<i>Index</i>	441

## Foreword

This is an impressive book by Wei Cai. It attempts to cover a wide range of topics in electromagnetics and electronic transport. In electromagnetics, it starts with low-frequency solutions of Poisson–Boltzmann equations that find wide applications in electrochemistry, in the interaction between electromagnetic fields and biological cells, as well as in the drift-diffusion model for electronic transport. In addition to low-frequency problems, the book also addresses wave physics problems of electromagnetic scattering, and the Schrödinger equation. It deals with dyadic Green’s function of layered media and relevant numerical methods such as surface integral equations, and finite element, finite difference, and discontinuous Galerkin methods. It also addresses interesting problems involving surface plasmons and periodic structures, as well as wave physics in the quantum regime.

In terms of quantum transport, the book discusses the non-equilibrium Green’s function method, which is a method currently in vogue. The book also touches upon hydrodynamic electron transport and the germane numerical methods.

This is an excellent book for those who want to study and understand the relationship between mathematical methods and the many different physical problems they can model and solve.

Weng Cho Chew, First Y. T. Lo Endowed Chair Professor, UIUC

## Preface

工若善其事，必先利其器

-Analects

Electromagnetic (EM) processes play an important role in many scientific and engineering applications such as the electrostatic forces in biomolecular solvation, radar wave scattering, the interaction of light with electrons in metallic materials, and current flows in nano-electronics, among many others. These are the kinds of electromagnetic phenomena, from atomistic to continuum scales, discussed in this book.

While the focus of the book is on a wide selection of various numerical methods for modeling electromagnetic phenomena, as listed under the entry “numerical methods” in the book index, attention is also given to the underlying physics of the problems under study. As computational research has become strongly influenced by the interaction from many different areas such as biology, physics, chemistry, and engineering, etc., a multi-faceted and balanced approach addressing the interconnection among mathematical algorithms and physical principles and applications is needed to prepare graduate students in applied mathematics, sciences, and engineering, to whom this book is aimed, for innovative advanced computational research.

This book arises from courses and lectures the author gave in various universities: the UNC Charlotte and the UC Santa Barbara in the USA, and Peking University, Fudan University, and Shanghai Jiao Tong University in China, to graduate students in applied mathematics and engineering. While attempts are made to include the most important numerical methods, the materials presented are undoubtedly affected by the author’s own research experience and knowledge. The principle of selecting the materials is guided by Confucius’s teaching above – “For a man to succeed in his endeavors, he must first sharpen his tools.” So, emphasis is on the practical and algorithmic aspects of methods ready for applications, instead of detailed and rigorous mathematical elucidation.

The book is divided into three major parts according to three broadly defined though interconnected areas: electrostatics in biomolecules, EM scattering and guiding in microwave and optical systems, and electron transport in semiconductor and plasma media. The first two areas are based on atomistic and continuum

EM theory, while the last one is based on Schrödinger quantum and also Maxwell EM theories. Part I starts with a chapter on the statistical molecular theory of dielectric constants for material polarization in response to an electric field, an important quantity for molecular dynamics simulation of biomolecules and understanding optical properties of materials addressed in the book. Then, the Poisson–Boltzmann (PB) theory for solvation is given in Chapter 2, together with analytical approximation methods such as the generalized Born method for solvation energy and image methods for reaction fields in simple geometries. Chapter 3 contains various numerical methods for solving the linearized PB equations including the boundary integral equation methods, the finite element methods, and the immersed interface methods. Chapter 4 presents three methods to handle the long-range electrostatic interactions – a key computational task in molecular dynamics algorithms: the particle-mesh Ewald, the fast multipole method, and a reaction field based hybrid method.

Part II contains a large collection of numerical techniques for solving the continuum Maxwell equations for scattering and propagation in time- and frequency-domains. This part starts with Chapter 5 on Maxwell equations with physical and artificial boundary conditions; the former includes dielectric interface conditions and Leontovich impedance boundary conditions for conductors with a perfect electric conductor (PEC) as a limiting case, and the latter includes local absorbing boundary conditions and uniaxial perfectly matched layer (PML) boundary conditions. Chapter 6 discusses the dyadic Green’s functions in layered media for the Maxwell equations in the frequency-domain and an algorithm for fast computation. High-order surface integral methods for electromagnetic scattering form the subject of Chapter 7, which includes the Galerkin method using mixed vector–scalar potentials and the Nyström collocation method for both the hyper-singular integral equations and the mixed vector–scalar potential integral equations, and combined integral equations for the removal of resonance in cavities. Finally, the high-order surface current basis for the Galerkin integral equation methods is discussed. Chapter 8 on edge elements begins with Nédélec’s original construction of the  $H(\text{curl})$  conforming basis, and then presents hierarchical high-order elements in 2-D rectangles and 3-D cubes and simplexes in both 2-D and 3-D spaces. Next, time-domain methods, including the discontinuous Galerkin (DG) methods with a high-order hierarchical basis and the finite difference Yee scheme, are given in Chapter 9. Numerical methods for periodic structures and surface plasmons in metallic systems are covered in Chapter 10, including plane-wave-based methods and transmission spectra calculations for photonics band structures, finite element methods, and volume integral equation (VIE) methods for the Maxwell equations. For the surface plasmons, the DG methods for dispersive media using auxiliary differential equations (ADEs) are given for Debye and Drude media. The final chapter (Chapter 11) of Part II contains numerical methods for Schrödinger equations for dielectric optical waveguides and quantum dots: a generalized DG method for the paraxial approximation in optical waveguides, and a VIE method

for Schrödinger equations in quantum dots embedded in layered semiconductor materials.

Part III starts with Chapter 12 on the electron quantum transport models in semiconductors, which also includes the Fermi–Dirac distribution for electron gas within the Gibbs ensemble theory, density operators, and kinetic descriptions for quantum systems. The quantum transport topics discussed in this chapter include the Wigner transport model in phase space for electrons, the Landauer transmission formula for quantum transport, and the non-equilibrium Green’s function (NEGF) method. Then, the non-equilibrium Green’s function method in Chapter 13 contains the treatment of quantum boundary conditions and finite difference and finite element methods for the NEGF; the latter allows the calculation of the transmission coefficients in the Landauer current formula for general nano-devices. Chapter 14 includes numerical methods for the quantum kinetic Wigner equations with the upwinding finite difference and an adaptive cell average spectral element method. Chapter 15 first presents the semi-classical Boltzmann and continuum hydrodynamic models for multi-species transport, including electron transport, and then follows with the numerical methods for solving the hydrodynamic equations by Godunov methods and WENO and central differencing methods. In the final chapter of the book, Chapter 16, we first present the kinetic Vlasov–Fokker–Planck (VFP) model and the continuum magneto-hydrodynamic (MHD) transport model for electrons in plasma media. Then, several numerical methods are discussed including the VFP scheme in phase space, and the particle-in-cell and constrained transport methods for the MHD model, where the divergence-free condition for the magnetic field is specifically enforced.

In making this book a reality, I credit my education and ways of doing research to my teachers Prof. Zhongci Shi at the University of Science and Technology of China (USTC), who exposed me to the power of non-conforming finite element methods and reminded me that computational research must not be devoid of real science and engineering relevance, and Prof. David Gottlieb (my doctoral thesis advisor) at Brown University, who taught me that simplicity is the beauty in sciences. Also, my scientific research has benefited greatly from encouragements and interactions from the late Prof. Steven Orszag over many years. I have learnt much from interactions with my colleague physicist Prof. Raphael Tsu (a co-inventor of the resonant tunneling diode and a pioneer in quantum superlattices), whose sharp physics insight has always been an inspiration and pleasure during many of our discussions. My former colleague Prof. Boris Rozovsky has provided much encouragement, spurring me to undertake the challenge of writing this book, which started in 2004 during one of my many research collaboration visits with Prof. Pingwen Zhang at Peking University through the Beijing International Center for Mathematical Research. This book would not be possible without the joint research work undertaken in the past few decades with my colleagues Pingwen Zhang and Shaozhong Deng, and my former students and postdoctoral researchers Tiejun Yu, Yijun Yu, Yuchun Lin, Tiao Lu, Xia Ji,



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