

# Contents

## Part I Collision Theory

<b>1</b>	<b>Potential Scattering</b> .....	3
1.1	Scattering by a Short-Range Potential .....	4
1.2	Scattering by a Coulomb Potential .....	10
1.3	Analytic Properties of the $S$ -Matrix .....	16
1.4	Effective Range Theory .....	23
1.4.1	Short-Range Potentials .....	23
1.4.2	Long-Range Potentials .....	29
1.4.3	Coulomb Potential .....	35
1.5	Variational Principles .....	41
1.6	Relativistic Scattering: The Dirac Equation .....	45
<b>2</b>	<b>Multichannel Collision Theory</b> .....	57
2.1	Wave Equation and Cross Section .....	58
2.2	Target Eigenstates and Pseudostates .....	60
2.2.1	Target Eigenstates .....	60
2.2.2	Target Pseudostates .....	64
2.3	Close Coupling Equations .....	69
2.3.1	Foundations of the Method .....	69
2.3.2	Derivation of the Close Coupling Equations .....	74
2.4	$K$ -Matrix and Kohn Variational Principle .....	84
2.5	$S$ -Matrix, $T$ -Matrix and Cross Sections .....	91
<b>3</b>	<b>Resonances and Threshold Behaviour</b> .....	101
3.1	Analytic Properties of the $S$ -Matrix .....	102
3.2	Bound States and Resonances .....	109
3.2.1	Bound-State and Resonance Poles in the $S$ -Matrix .....	110
3.2.2	Behaviour of the $S$ -Matrix Near a Resonance .....	112
3.2.3	Behaviour of Eigenphases Near a Resonance .....	117
3.2.4	Time-Delay Matrix .....	121

3.2.5	Feshbach Projection Operator Theory	125
3.2.6	Hyperspherical Coordinates	129
3.3	Threshold Behaviour of Cross Sections	135
3.3.1	Excitation: Short-Range Potentials	135
3.3.2	Excitation: Dipole Potentials	139
3.3.3	Excitation: Coulomb Potential	145
3.3.4	Multichannel Quantum Defect Theory	151
3.3.5	Threshold Behaviour of Ionization	159

## Part II R-Matrix Theory and Applications

<b>4</b>	<b>Introduction to R-Matrix Theory: Potential Scattering</b>	167
4.1	Wigner–Eisenbud Theory	170
4.2	Generalized <i>R</i> -Matrix Theory	175
4.3	Variational Principles for the <i>R</i> -Matrix	179
4.4	<i>R</i> -Matrix Approximation Methods	181
4.4.1	Homogeneous Boundary Condition Method	181
4.4.2	Buttle Corrections to the <i>R</i> -Matrix and Wave Function	184
4.4.3	Arbitrary Boundary Condition Methods	187
4.4.4	Linear Equations Method	191
4.4.5	Eigenchannel Methods	192
4.4.6	Lagrange Mesh Methods	197
4.4.7	B-Spline Methods	201
4.4.8	Direct Calculation of Siegert State Parameters	207
4.5	Propagator Methods	209
4.5.1	Light–Walker Propagator	210
4.5.2	BBM Propagator	213
4.6	Dirac <i>R</i> -Matrix Theory	215
<b>5</b>	<b>Electron Collisions with Atoms and Ions</b>	227
5.1	Multichannel <i>R</i> -Matrix Theory	228
5.1.1	Introduction and Computer Programs	229
5.1.2	Internal Region Solution	232
5.1.3	External Region Solution	238
5.1.4	Asymptotic Region Solution	240
5.2	Variational Principle for the <i>R</i> -Matrix	242
5.3	Continuum Basis Orbitals and Correction Methods	247
5.3.1	Homogeneous Boundary Condition Method	248
5.3.2	Buttle Correction to the <i>R</i> -Matrix and Wave Function	250
5.3.3	Arbitrary Boundary Condition Methods	254
5.3.4	Partitioned <i>R</i> -Matrix Method	256
5.4	Inclusion of Relativistic Effects	260
5.4.1	Transformation of the <i>K</i> - and <i>S</i> -Matrices	261
5.4.2	Breit–Pauli Hamiltonian	265
5.4.3	Frame-Transformation Theory	272

5.5	Dirac <i>R</i> -Matrix Theory . . . . .	275
5.5.1	Introduction and Computer Programs . . . . .	276
5.5.2	Internal Region Solution . . . . .	277
5.5.3	External Region Solution . . . . .	284
5.5.4	Asymptotic Region Solution . . . . .	287
5.5.5	Continuum Basis Orbitals . . . . .	289
5.5.6	Buttle Correction . . . . .	291
5.6	Low-Energy Electron Collision Calculations . . . . .	292
5.6.1	Electron Collisions with H . . . . .	292
5.6.2	Electron Collisions with He . . . . .	294
5.6.3	Electron Collisions with Ne . . . . .	298
5.6.4	Electron Collisions with Si III . . . . .	299
5.6.5	Electron Collisions with Fe II . . . . .	301
5.6.6	Electron Collisions with Fe XV . . . . .	307
5.6.7	Electron Collisions with Xe XXVII . . . . .	309
<b>6</b>	<b>Intermediate-Energy Collisions . . . . .</b>	<b>311</b>
6.1	Overview of Intermediate-Energy Methods . . . . .	312
6.2	<i>R</i> -Matrix with Pseudostates Method . . . . .	316
6.3	Intermediate-Energy <i>R</i> -Matrix Method . . . . .	322
6.3.1	General Procedure . . . . .	323
6.3.2	Two-Electron Example . . . . .	327
6.4	<i>T</i> -Matrix Energy Averaging . . . . .	337
6.5	Distorted Wave and Second-Born Methods . . . . .	343
6.6	Intermediate-Energy Electron Collision Calculations . . . . .	348
6.6.1	Electron Collisions with H . . . . .	348
6.6.2	Electron Collisions with C IV . . . . .	351
6.6.3	Electron Impact Excitation–Ionization of He . . . . .	352
<b>7</b>	<b>Positron Collisions with Atoms and Ions . . . . .</b>	<b>355</b>
7.1	Multichannel <i>R</i> -Matrix Theory . . . . .	356
7.1.1	Introduction . . . . .	356
7.1.2	Internal Region Solution . . . . .	360
7.1.3	External Region Solution . . . . .	367
7.1.4	Asymptotic Region Solution . . . . .	370
7.2	Positron and Positronium Collision Calculations . . . . .	373
7.2.1	Positron Collisions with H . . . . .	373
7.2.2	Positronium Collisions with He . . . . .	375
7.2.3	Target Polarization in Positronium Collisions . . . . .	377
<b>8</b>	<b>Photoionization, Photorecombination and Atoms in Fields . . . . .</b>	<b>379</b>
8.1	Atomic Photoionization . . . . .	380
8.1.1	Introduction and General Theory . . . . .	380
8.1.2	<i>R</i> -Matrix Theory . . . . .	390

8.2	Photorecombination and Radiation Damping . . . . .	404
8.2.1	Introduction . . . . .	404
8.2.2	<i>R</i> -Matrix Theory . . . . .	406
8.3	The Opacity Project . . . . .	414
8.4	Spectra of Atoms in Fields . . . . .	416
8.5	Illustrative Examples . . . . .	422
8.5.1	Photoionization of Li . . . . .	423
8.5.2	Photoionization of Fe VII . . . . .	424
8.5.3	Photorecombination in Electron Collisions with O VIII . . . . .	426
8.5.4	Radiation Damping in Electron Collisions with Fe XXVI . . . . .	428
8.5.5	Radiation Damping in Electron Collisions with W XLVII . . . . .	428
8.5.6	Photoionization Spectrum of Li in a Magnetic Field . . . . .	431
<b>9</b>	<b>Multiphoton Processes: Floquet Theory . . . . .</b>	<b>433</b>
9.1	<i>R</i> -Matrix–Floquet Theory . . . . .	434
9.1.1	Introduction . . . . .	434
9.1.2	Internal Region Solution . . . . .	436
9.1.3	External Region Solution . . . . .	441
9.1.4	Asymptotic Region Solution in the Velocity Gauge . . . . .	451
9.1.5	Asymptotic Region Solution in the Acceleration Frame . . . . .	456
9.1.6	Asymptotic Region Solution: Simplified Analysis . . . . .	466
9.1.7	Harmonic Generation . . . . .	473
9.1.8	Non-hermitian Floquet Dynamics . . . . .	477
9.2	Illustrative Examples . . . . .	480
9.2.1	Resonances in Multiphoton Ionization . . . . .	480
9.2.2	Harmonic Generation . . . . .	484
9.2.3	Laser-Induced Degenerate States . . . . .	487
9.2.4	Laser-Assisted Electron–Atom Collisions . . . . .	489
<b>10</b>	<b>Multiphoton Processes: Time-Dependent Theory . . . . .</b>	<b>493</b>
10.1	Time-Dependent <i>R</i> -Matrix Theory . . . . .	494
10.1.1	Introduction . . . . .	494
10.1.2	Internal Region Solution . . . . .	499
10.1.3	External Region Solution . . . . .	506
10.1.4	Computational Methods . . . . .	511
10.1.5	Analysis of Applications . . . . .	516
10.2	Illustrative Examples . . . . .	523
10.2.1	Multiphoton Ionization of Ne . . . . .	524
10.2.2	Multiphoton Ionization of Ar . . . . .	528

<b>11 Collisions with Molecules</b> .....	533
11.1 Electron Collisions with Molecules .....	535
11.1.1 Introduction .....	535
11.1.2 Fixed-Nuclei <i>R</i> -Matrix Theory .....	536
11.1.3 Inclusion of Nuclear Motion .....	544
11.1.4 Non-adiabatic <i>R</i> -Matrix Theory .....	548
11.1.5 Resonant <i>R</i> -Matrix Theory .....	560
11.1.6 Scattering Amplitudes and Cross Sections .....	561
11.1.7 Illustrative Examples: N <sub>2</sub> , O <sub>2</sub> , N <sub>2</sub> O, H <sub>3</sub> <sup>+</sup> .....	566
11.2 Positron Collisions with Molecules .....	573
11.2.1 <i>R</i> -Matrix Theory and Calculations .....	573
11.2.2 Illustrative Examples: H <sub>2</sub> O, CO <sub>2</sub> .....	575
11.3 Molecular Multiphoton Processes .....	579
11.3.1 Molecular <i>R</i> -Matrix–Floquet Theory .....	579
11.3.2 Illustrative Example: H <sub>2</sub> .....	588
<b>12 Electron Interactions in Solids</b> .....	591
12.1 Electron Collisions with Transition Metal Oxides .....	592
12.1.1 Introduction .....	592
12.1.2 <i>R</i> -Matrix Theory .....	592
12.1.3 Illustrative Example .....	594
12.2 Electron Transport in Semiconductor Devices .....	596
12.2.1 Introduction .....	596
12.2.2 <i>R</i> -Matrix Theory .....	597
12.2.3 Illustrative Example .....	602
<b>Part III Appendices</b>	
<b>Appendix A Clebsch–Gordan and Racah Coefficients</b> .....	607
A.1 Clebsch–Gordan Coefficients .....	607
A.2 Racah Coefficients .....	612
A.3 6- <i>j</i> Symbols .....	615
A.4 9- <i>j</i> Symbols .....	615
A.5 Higher Order 3 <i>n</i> - <i>j</i> Symbols .....	617
<b>Appendix B Legendre Polynomials and Related Functions</b> .....	619
B.1 Legendre Polynomials .....	619
B.2 Associated Legendre Functions .....	621
B.3 Spherical Harmonics .....	623
B.4 Phase of Spherical Harmonics .....	628
B.5 Transformation Under Rotations .....	632

<b>Appendix C</b>	<b>Bessel Functions and Related Functions</b>	639
C.1	Bessel Functions	639
C.2	Spherical Bessel Functions	642
<b>Appendix D</b>	<b>Applications of Angular Momentum Algebra</b>	647
D.1	Long-Range Electron–Atom Potential Coefficients	647
D.1.1	Non-relativistic Collisions	647
D.1.2	Inclusion of Relativistic Effects	652
D.2	<i>R</i> -Matrix–Floquet Multiphoton Potential	654
D.3	Time-Dependent Multiphoton Potential	657
D.4	Atomic Photoionization Cross Section	662
<b>Appendix E</b>	<b>Propagator Methods</b>	665
E.1	Light–Walker Propagator Method	666
E.2	Log-Derivative Propagator Method	671
E.3	BBM Propagator Method	675
E.4	Propagation of Driven Equations	678
E.5	Propagator Method with First-Order Derivative	681
E.6	Propagation of Sets of Uncoupled Channels	684
<b>Appendix F</b>	<b>Asymptotic Expansions</b>	693
F.1	Electron and Positron Collisions	693
F.2	Multiphoton Processes	700
<b>References</b>		707
<b>Index</b>		731