

---

## Contents

---

### Part I Relativity in atomic and molecular physics

---

<b>1</b>	<b>Relativity in atomic and molecular physics</b>	<b>3</b>
1.1	Elementary ideas	3
1.2	The one-electron atom	7
1.2.1	Classical Kepler orbits	7
1.2.2	The Bohr atom	8
1.2.3	X-ray spectra and Moseley's Law	9
1.2.4	Transition to quantum mechanics	9
1.2.5	Sommerfeld's relativistic orbits and Dirac's wave equation	10
1.2.6	Dirac and Schrödinger charge distributions	13
1.2.7	The Dirac hydrogenic spectrum at high $Z$	17
1.3	Many-electron atoms	19
1.3.1	Central field models of the atom	20
1.3.2	Closed and open shells	21
1.3.3	Mean field potentials	23
1.3.4	Comparison of Hartree-Fock and Dirac-Hartree-Fock models for ground states	24
1.3.5	The mechanism of shell filling	35
1.3.6	Other approaches	38
1.4	Applications to atomic physics	40
1.4.1	X-ray spectra	41
1.4.2	Applications to astrophysics and plasma physics	43
1.4.3	Modelling atomic processes in plasmas	44
1.5	Relativistic molecular structure	45
1.5.1	Relativistic interpretations of chemical anomalies	46
1.5.2	Relativistic effective core potentials and other approximations	48
1.5.3	Dirac four-component methods for molecules	51

1.5.4	Parity violation and hyperfine interactions .....	52
1.5.5	High-precision spectroscopy of small molecules containing light elements .....	54
<b>References</b> .....		54

**Part II Foundations**

<b>2</b>	<b>Relativistic wave equations for free particles</b> .....	63
2.1	The special theory of relativity .....	63
2.2	The Lorentz group .....	66
2.2.1	* Spinor representation of Lorentz transformations .....	67
2.2.2	* Infinitesimal Lorentz transformations and their generators .....	69
2.2.3	* Representations of the Lorentz group .....	70
2.3	The Poincaré group .....	73
2.3.1	* Representations of the Poincaré group .....	75
2.3.2	* Space and time reflections .....	77
2.4	The Klein-Gordon equation .....	81
2.5	The Dirac equation .....	86
2.5.1	$\gamma$ -Matrices and covariant form of Dirac's equation .....	87
2.5.2	* Lagrangian formulation of Dirac's equation .....	88
2.5.3	Foldy canonical form and the Foldy-Wouthuysen transformation .....	90
2.5.4	* Position operators in Dirac theory .....	92
2.5.5	Dirac particles in electromagnetic fields .....	94
2.5.6	* Negative energy states .....	95
2.6	Maxwell's equations .....	96
2.6.1	Covariant form of Maxwell's equations .....	96
2.6.2	* Lagrangian formulation .....	99
2.6.3	Gauge invariance .....	100
2.6.4	* Motion of a test charge .....	102
2.7	* Symmetries and local conservation laws .....	103
2.8	* Global conservation laws .....	107
2.9	* Green's functions .....	108
2.9.1	Nonrelativistic Green's functions .....	109
2.9.2	Klein-Gordon operator .....	112
2.9.3	Maxwell's equations: the zero-mass case .....	116
2.9.4	Free-particle Dirac equation .....	118
<b>References</b> .....		119

<b>3</b>	<b>The Dirac Equation</b> .....	121
3.1	Free particles .....	121
3.1.1	Properties of Dirac matrices .....	122
3.1.2	Covariance properties .....	123
3.1.3	Bilinear covariants .....	125
3.1.4	Plane wave solutions .....	126
3.1.5	Energy and spin projectors .....	128
3.1.6	Charge conjugation .....	130
3.2	Spherical symmetry .....	132
3.2.1	Angular structure .....	133
3.2.2	The operator $\sigma_r$ .....	134
3.2.3	The operator $c\boldsymbol{\sigma} \cdot \mathbf{p}$ .....	136
3.2.4	Separation of radial and spin-angular parts .....	136
3.2.5	Angular density distributions .....	137
3.2.6	Radial solutions for the free particle .....	141
3.2.7	Partial wave normalization .....	142
3.3	Hydrogenic atoms .....	143
3.3.1	Solution of the radial equations .....	146
3.3.2	The bound state solutions .....	148
3.3.3	Charge distributions and energy levels in hydrogenic atoms .....	149
3.3.4	* The continuum solutions .....	150
3.4	Scattering by a centre of force .....	152
3.4.1	Nonrelativistic potential scattering .....	152
3.4.2	* Relativistic Coulomb scattering .....	155
3.4.3	* Polarization effects in Coulomb scattering .....	158
3.4.4	Historical note .....	160
3.5	* Relativistic quantum defect theory .....	161
3.6	Green's functions .....	166
3.6.1	* Partial wave Green's functions .....	167
3.6.2	The partial wave Green's function for the free Dirac particle .....	169
3.6.3	Summation over partial waves in the free electron case .....	170
3.6.4	* Green's function for hydrogenic ions .....	171
3.7	The nonrelativistic limit: the Pauli approximation .....	173
3.7.1	The Pauli approximation .....	173
3.7.2	The Foldy-Wouthuysen and related transformations .....	175
3.8	Other aspects of Dirac theory .....	178
<b>References</b> .....		178
<b>4</b>	<b>Quantum electrodynamics</b> .....	181
4.1	Second quantization .....	181
4.1.1	Quantization of the Schrödinger equation .....	181
4.1.2	Identical particles: the symmetric case .....	184

4.1.3 Identical particles: the antisymmetric case . . . . .	188
4.2 Quantization of the electron-positron field . . . . .	189
4.2.1 The Furry picture . . . . .	189
4.2.2 The free electron case . . . . .	192
4.3 Quantization of the Maxwell field . . . . .	196
4.4 Interaction of photons and electrons . . . . .	200
4.4.1 The equations of motion . . . . .	200
4.4.2 The Furry picture . . . . .	202
4.4.3 The interaction picture . . . . .	203
4.5 Wick's theorems . . . . .	206
4.6 Propagators . . . . .	208
4.6.1 Photon propagators . . . . .	208
4.6.2 Electron-positron propagators . . . . .	209
4.6.3 Feynman diagrams . . . . .	210
4.6.4 Second order interaction: $U^{(2)}(t, t_0)$ . . . . .	212
4.6.5 Feynman rules . . . . .	216
4.7 The S-matrix . . . . .	217
4.8 Bound states . . . . .	218
4.8.1 A perturbation expansion . . . . .	218
4.8.2 Gell-Mann, Low, Sucher energy shift . . . . .	219
4.9 Effective interactions . . . . .	222
4.9.1 One-photon exchange: Feynman gauge . . . . .	222
4.9.2 One-photon exchange: Coulomb gauge . . . . .	225
4.9.3 * Off-shell potentials: heuristic argument . . . . .	227
4.9.4 One-photon exchange: the first order energy shift . . . . .	227
4.10 * Off-shell potentials . . . . .	228
4.11 Many-body perturbation theory . . . . .	232
4.11.1 Nonrelativistic many-body theory . . . . .	233
4.12 MBPT for atoms and molecules . . . . .	236
4.12.1 Particle-hole formalism . . . . .	236
4.12.2 Computational methods . . . . .	238
4.13 Relativistic approaches to atomic and molecular structure . . . . .	238
4.13.1 The no-virtual-pair approximation (NVPA) . . . . .	238
4.13.2 The NVPA as an antidote to “continuum dissolution” . . . . .	239
4.13.3 The NVPA and “variational collapse” . . . . .	242
4.13.4 Semirelativistic approaches . . . . .	243
4.14 A strategy for atomic and molecular calculations . . . . .	243
4.15 Density functional theories . . . . .	245
4.15.1 Basic ideas of RDFT . . . . .	246
4.15.2 The relativistic Hohenberg-Kohn theorem . . . . .	247
4.15.3 The relativistic Kohn-Sham equations . . . . .	248
4.15.4 Exchange and correlation functionals . . . . .	249
4.15.5 The optimized potential method . . . . .	252
References . . . . .	253

---

### Part III Computational atomic and molecular structure

---

5 Analysis and approximation of Dirac Hamiltonians . . . . .	259
5.1 Self-adjointness of free particle Hamiltonians . . . . .	260
5.1.1 Free particles: the Schrödinger case . . . . .	260
5.1.2 Free particles: the Dirac case . . . . .	261
5.2 Self-adjointness of Hamiltonians with a local potential . . . . .	262
5.2.1 The Schrödinger case . . . . .	263
5.2.2 The Dirac case . . . . .	264
5.3 The radial Dirac differential operator . . . . .	265
5.3.1 The boundary condition at a singular endpoint . . . . .	266
5.3.2 The Dirac radial operator with one singular endpoint . . . . .	267
5.4 The radial Dirac equation for atoms . . . . .	270
5.4.1 Power series solutions near $r = 0$ . . . . .	272
5.4.2 Power series solutions in the nonrelativistic limit . . . . .	273
5.4.3 The boundary condition at the origin . . . . .	274
5.5 Variational methods in quantum mechanics . . . . .	274
5.5.1 Min-max theorems and the Ritz method . . . . .	276
5.5.2 Convergence of the Rayleigh-Ritz eigenvalues in nonrelativistic quantum mechanics . . . . .	279
5.5.3 Convergence of the Rayleigh-Ritz method in nonrelativistic quantum mechanics . . . . .	283
5.6 The Rayleigh-Ritz method in relativistic quantum mechanics . . . . .	285
5.6.1 The finite matrix method for the Dirac equation . . . . .	285
5.6.2 Convergence of Rayleigh-Ritz methods for Dirac Hamiltonians . . . . .	287
5.7 Spinor basis sets . . . . .	290
5.8 L-spinors . . . . .	293
5.8.1 Kinetic matching and the nonrelativistic limit . . . . .	295
5.8.2 Orthogonality properties . . . . .	295
5.8.3 Linear independence of L-spinors . . . . .	296
5.8.4 Completeness of L-spinors . . . . .	297
5.8.5 Charge conjugation and L-spinors . . . . .	297
5.8.6 Construction of $\boldsymbol{\Pi}^{\beta\beta'}$ , $\mathbf{S}^{\beta\beta'}$ , and $\mathbf{U}^{\beta\beta'}$ matrices for hydrogenic atoms . . . . .	298
5.8.7 Numerical study of L-spinor performance in hydrogenic atoms . . . . .	299
5.9 S-spinors . . . . .	303
5.9.1 Construction of $\boldsymbol{\Pi}^{\beta\beta'}$ , $\mathbf{S}^{\beta\beta'}$ , and $\mathbf{U}^{\beta\beta'}$ for hydrogenic atoms . . . . .	304
5.10 G-spinors . . . . .	305
5.11 Finite difference methods . . . . .	307
5.11.1 Methods of solution . . . . .	309

5.11.2 Acceptable solutions .....	312
5.12 Finite element methods .....	315
5.12.1 B-splines .....	316
5.12.2 Variational formulation of finite element schemes .....	316
5.12.3 Schrödinger equations .....	318
5.12.4 Dirac equations .....	319
<b>References .....</b>	<b>322</b>
<b>6 Complex atoms .....</b>	<b>325</b>
6.1 Dirac-Hartree-Fock theory .....	325
6.2 One-electron matrix elements of tensor operators .....	327
6.2.1 2-spinor matrix elements of even operators.....	328
6.2.2 2-spinor matrix elements of odd operators .....	330
6.3 Angular reduction of the Dirac Hamiltonian for a central potential .....	331
6.4 Matrix elements of 2-body operators .....	333
6.4.1 The Coulomb interaction .....	333
6.4.2 Relativistic corrections to the Coulomb interaction .....	334
6.4.3 The Gaunt interaction .....	335
6.4.4 The Møller interaction .....	336
6.4.5 The transverse photon interaction in Coulomb gauge...	337
6.4.6 The Breit interaction .....	339
6.5 Interaction strengths for the magnetic interactions .....	340
6.5.1 The transverse photon interaction .....	340
6.5.2 The Breit interaction .....	344
6.6 Closed shells and configuration averages .....	346
6.6.1 The Dirac-Hartree-Fock model .....	346
6.6.2 Inclusion of magnetic interactions .....	349
6.6.3 Average of configuration models .....	350
6.7 DHF integro-differential equations .....	352
6.7.1 Construction of electrostatic potentials .....	356
6.7.2 Construction of magnetic potentials .....	356
6.7.3 Algorithms for potentials and Slater integrals .....	359
6.8 Configurations with incomplete subshells .....	361
6.8.1 Atomic states with incomplete subshells .....	361
6.8.2 Partially filled subshells in $jj$ -coupling .....	363
6.8.3 Creation and annihilation operators as irreducible tensor operators. Quasispin. ....	364
6.8.4 Double tensor operators .....	366
6.8.5 Parentage .....	367
6.8.6 Coefficients of fractional parentage in the seniority scheme .....	370
6.8.7 Equivalent electrons in $LS$ -coupling.....	374
6.9 Atoms with complex configurations .....	376

6.9.1 Recoupling coefficients .....	379
6.9.2 Matrix elements between open shell states .....	379
6.9.3 Matrix elements of two-electron operators of type $\mathbf{G}$ .....	382
6.10 CI and MCDHF problems with large CSF sets .....	384
6.10.1 Decoupling active electrons .....	385
6.10.2 One-electron matrix elements .....	388
6.10.3 Two-electron matrix elements .....	388
<b>References .....</b>	<b>391</b>
<b>7 Computation of atomic structures .....</b>	<b>393</b>
7.1 Atomic structure calculations with GRASP .....	393
7.2 GRASP modules .....	394
7.3 MCDHF integro-differential equations .....	398
7.4 Solving the integro-differential equations .....	401
7.5 Starting the calculation .....	403
7.5.1 The radial grid .....	403
7.5.2 The nuclear mass .....	405
7.5.3 The nuclear size .....	405
7.5.4 Initial estimates for radial wavefunctions .....	406
7.6 An EAL calculation .....	407
7.7 Diagonal and off-diagonal energy parameters .....	408
7.8 Koopmans' theorem and Brillouin's theorem .....	411
7.8.1 Froese Fischer's analysis .....	412
7.9 Control of MCSCF iterations .....	416
7.10 Corrections to the Coulomb interaction: Breit and other approximations.....	418
7.11 QED corrections .....	419
7.12 Towards higher quality atomic models .....	423
7.12.1 CSF sets for electron correlation: active space methods ..	424
7.12.2 Example: intercombination transitions in Be-like ions ..	426
7.13 X-ray transition energies .....	428
<b>References .....</b>	<b>431</b>
<b>8 Computation of atomic properties .....</b>	<b>433</b>
8.1 Relativistic radiative transition theory .....	433
8.1.1 Line transitions .....	433
8.1.2 Multipole expansion of the radiation field .....	434
8.2 Emission and absorption by one-electron atoms .....	437
8.2.1 Evaluation of one-electron transition amplitudes .....	439
8.2.2 The nonrelativistic limit: Pauli approximation .....	440
8.3 Radiative transitions in many-electron atoms .....	443
8.3.1 Transitions in highly ionized atoms: Fe XXIII .....	443
8.4 Orbital relaxation .....	444

8.5 Application to atomic transition calculations .....	448
8.5.1 Large-scale calculations of energies and transition rates .....	451
8.6 Relativistic atomic photo-ionization theory .....	452
8.6.1 The differential cross-section for photo-ionization .....	453
8.6.2 Low energies: the electric dipole case .....	455
8.6.3 Angular distributions and polarization parameters for a single channel .....	457
8.6.4 Other aspects of photo-ionization .....	458
8.7 Hyperfine interactions .....	459
8.7.1 Hyperfine interactions in the many-electron atom .....	461
8.8 Isotope shifts .....	464
8.8.1 Nuclear motion .....	464
8.8.2 Nuclear volume effect .....	466
<b>References</b> .....	467
<b>9 Continuum processes in many-electron atoms</b> .....	471
9.1 Relativistic elastic electron-atom scattering .....	471
9.1.1 Model potentials .....	473
9.1.2 Computational issues .....	473
9.1.3 Other approaches .....	474
9.1.4 Determination of phase-shifts .....	475
9.1.5 Summation of the partial wave expansion .....	477
9.2 Electron-atom scattering: the close-coupling method .....	477
9.2.1 Low-energy elastic and inelastic collisions .....	477
9.2.2 The distorted wave approximation .....	480
9.3 The relativistic R-matrix method .....	480
9.3.1 The radial Dirac equation on a finite interval .....	481
9.3.2 Bloch operators .....	483
9.3.3 The inner region, $r \leq a$ .....	485
9.3.4 The outer region, $r > a$ .....	489
9.3.5 Matching inner and outer solutions .....	489
9.4 The Buttle correction .....	492
9.5 R-matrix theory of photo-ionization .....	493
9.6 The DARC relativistic R-matrix package .....	494
9.7 Truncation of the close-coupling expansion. The nonrelativistic CCC method .....	496
9.8 The R-matrix method at intermediate energies .....	500
9.9 Electron scattering from heavy atoms and ions .....	504
9.9.1 Early work .....	504
9.9.2 Electron scattering from the mercury atom .....	505
9.9.3 Scattering of polarized electrons from polarized atoms .....	509
9.10 The relativistic random phase approximation .....	513
9.10.1 The RRPA equations .....	513
9.10.2 Radial equations .....	516

9.10.3 Multipole transition amplitudes .....	518
9.11 RRPA rates for photo-excitation and photo-ionization .....	520
9.11.1 Photo-excitation .....	520
9.11.2 Photo-ionization .....	520
9.12 Comparison with experiment .....	523
9.12.1 Photo-ionization of outer atomic subshells at high Z .....	523
9.12.2 Beyond RRPA .....	526
<b>References</b> .....	529
<b>10 Molecular structure methods</b> .....	533
10.1 Molecular and atomic structure methods .....	533
10.2 Dirac-Hartree-Fock-Breit equations for closed shell atoms .....	535
10.2.1 DHFB energy of a closed shell atom .....	535
10.2.2 Spinor basis function representation .....	535
10.2.3 Matrix of the radial Dirac operator .....	536
10.2.4 Coulomb Slater integrals .....	536
10.2.5 Breit integrals for closed shells .....	537
10.2.6 The DHFB Fock matrix .....	538
10.3 One-centre interaction integrals .....	539
10.4 Numerical examples .....	541
10.5 The DHFB method for closed shell molecules .....	543
10.6 G-spinor basis functions .....	544
10.7 The charge-current density .....	545
10.8 Two-centre overlaps .....	546
10.8.1 Relativistic expansion coefficients .....	547
10.8.2 Symmetry properties of $E_q$ coefficients .....	548
10.9 Multi-centre interaction integrals .....	549
10.9.1 Auxiliary integrals involving HGTFs .....	550
10.9.2 Multi-centre one-electron integrals .....	551
10.9.3 Multi-centre two-electron integrals .....	556
10.10 Fock matrix in terms of G-spinors .....	558
10.10.1 The BERTHA integral package .....	560
10.11 Electromagnetic field energy .....	562
10.11.1 Interaction energy in terms of internal fields .....	562
10.11.2 The nonrelativistic Fock matrix .....	565
10.11.3 The relativistic Fock matrix .....	565
10.11.4 Implementation of the field formulation .....	566
10.12 Relativistic density functional calculations .....	568
10.13 Computational strategies .....	574
10.13.1 The Roothaan bound .....	575
10.13.2 Integral-direct Fock matrix evaluation .....	575
10.13.3 Symmetry properties of interaction matrix elements .....	576
10.13.4 Stepwise refinement .....	576
10.13.5 Level-shifting .....	577

10.14 Multiconfigurational Dirac-Hartree-Fock theory .....	578
10.14.1 Orbital optimization .....	578
<b>References .....</b>	<b>584</b>
<b>11 Relativistic calculation of molecular properties .....</b>	<b>587</b>
11.1 Molecular symmetry .....	587
11.1.1 Diatomic molecules .....	589
11.1.2 Polyatomic molecules .....	591
11.2 Relativistic effects in light molecules .....	594
11.2.1 Nonrelativistic Breit-Pauli model .....	594
11.2.2 DHF and DHFB calculations for water using BERTHA .....	596
11.2.3 Second-order many-body corrections .....	598
11.2.4 Relativistic study of the potential energy surface and vibration-rotation levels of water .....	599
11.3 Electromagnetic properties of atoms and molecules .....	601
11.3.1 Gauge transformations in electromagnetic processes .....	601
11.3.2 B-spinors .....	602
11.4 The Zeeman effect .....	603
11.5 Hyperfine interactions .....	606
11.6 NMR shielding in small molecules .....	609
11.6.1 NMR shielding constants for $^{17}\text{O}$ in water .....	611
11.6.2 NMR shielding constants for $^{15}\text{N}$ in ammonia .....	612
11.7 Molecules with high-Z constituents .....	613
11.7.1 Electronic structure of $\text{TiF}$ .....	614
11.7.2 Electronic structure of $\text{YbF}$ .....	617
11.7.3 DHF+CI study of uranium hexafluoride .....	620
<b>References .....</b>	<b>624</b>
<b>A Frequently used formulae and data .....</b>	<b>627</b>
A.1 Relativistic notation .....	627
A.2 Dirac matrices .....	628
A.3 Special functions .....	631
A.3.1 Spherical Bessel functions .....	631
A.3.2 Confluent hypergeometric functions .....	632
A.3.3 Generalized Laguerre polynomials .....	633
A.3.4 Hermite polynomials .....	634
A.3.5 Incomplete gamma functions .....	635
A.3.6 Incomplete beta functions .....	635
A.3.7 Continued fraction evaluation .....	636
A.4 Central field Dirac spinors and their interactions .....	636
A.4.1 Central field Dirac spinors .....	636
A.4.2 Matrix elements of simple ITOs .....	639
A.4.3 Magnetic interactions .....	642

A.4.4 Effective interaction strengths for two-body operators .....	644
A.5 Open shells in $jj$ -coupling .....	651
A.6 Exponents for atomic and molecular G-spinors .....	654
A.7 Software for relativistic molecular calculations .....	662
A.7.1 BERTHA .....	662
A.7.2 DIRAC .....	662
A.7.3 MOLFDIR .....	663
<b>References .....</b>	<b>664</b>
<b>B Supplementary mathematics .....</b>	<b>665</b>
B.1 Linear operators on Hilbert space .....	665
B.1.1 Hilbert spaces .....	665
B.1.2 Linear operators .....	665
B.1.3 Spectrum and resolvent of linear operators .....	666
B.1.4 Self-adjoint operators .....	666
B.1.5 Observables and self-adjoint operators .....	669
B.1.6 Commuting operators .....	671
B.1.7 Unitary and anti-unitary operators .....	671
B.2 Lie groups and Lie algebras .....	673
B.2.1 Lie groups .....	673
B.2.2 Lie algebras .....	674
B.2.3 Representations of Lie groups and Lie algebras .....	676
B.2.4 The Cartan-Weyl classification .....	677
B.2.5 Casimir operators .....	678
B.2.6 Kronecker products of group representations .....	679
B.2.7 Tensor operators and the Wigner-Eckart theorem .....	681
B.3 Quantum mechanical angular momentum theory .....	683
B.3.1 The rotation group .....	683
B.3.2 Abstract angular momentum .....	684
B.3.3 Orbital angular momentum .....	685
B.3.4 Representation functions .....	687
B.3.5 Kronecker products of irreducible representations .....	691
B.3.6 Coupling of three or more angular momenta .....	693
B.3.7 The $3j$ -symbol .....	694
B.3.8 The $6j$ -symbol .....	694
B.3.9 The $9j$ -symbols .....	696
B.3.10 Graphical treatment of angular momentum algebra .....	697
B.3.11 Diagrammatic treatment of Clebsch-Gordan coefficients .....	699
B.3.12 Diagrammatic treatment of $3jm$ -symbols .....	701
B.3.13 Generalized angular momentum coupling schemes .....	703
B.3.14 GCG and $njm$ coefficients .....	706
B.3.15 Manipulating angular momentum diagrams .....	708
B.3.16 Tensor operators and the Wigner-Eckart theorem .....	709
B.3.17 Composite tensor operators .....	711

B.3.18	Diagrammatic representation of tensor operators	713
B.4	Relativistic symmetry orbitals for double point groups	717
B.4.1	Construction of symmetry orbitals	717
B.4.2	Linear independence of molecular symmetry orbitals	719
B.4.3	Reduction of operator matrices	719
B.4.4	Time reversal	720
B.4.5	The TSYM software package	722
B.5	Basis sets in atomic and molecular physics	722
B.5.1	The Coulomb Sturmian functions	727
B.5.2	Completeness and linear independence of Coulomb Sturmians	729
B.5.3	Basis sets of exponential-type functions	730
B.6	Finite difference methods for Dirac equations	733
B.6.1	An existence theorem	733
B.6.2	Initial value methods	734
B.6.3	Linear multistep methods	736
B.6.4	The nodal structure of Dirac radial wavefunctions	738
B.6.5	Discretization of two-point boundary value problems	741
B.6.6	Two-point boundary value problems: the deferred correction method	744
B.6.7	Construction of difference corrections	746
B.6.8	Single stepping algorithms	748
B.6.9	Stepping outwards from the origin	749
B.6.10	Algorithm for the outer region	751
B.6.11	The boundary condition at $T = t_N$	753
B.6.12	The boundary condition at the origin	754
B.6.13	Improving a trial solution	755
B.7	Eigenfunction expansions for the radially reduced Dirac equation	757
B.7.1	The fundamental lemma	757
B.7.2	Boundary conditions: the two-point boundary value problem	758
B.7.3	Boundary conditions at the nucleus	759
B.7.4	Pauli approximation at $R_2$	759
B.7.5	The MIT bag model at $R_2$	759
B.7.6	The eigenvalue spectrum	760
B.7.7	The inhomogeneous boundary value problem	761
B.7.8	Eigenfunction expansions	766
B.8	Iterative processes in nonlinear systems of equations	769
B.9	Lagrangian and Hamiltonian methods	772
B.9.1	Lagrange's equations	772
B.9.2	Hamilton's equations	773
B.9.3	Symmetries and conservation laws	775
B.10	Construction of $E$ coefficients	777
B.10.1	$E$ -coefficients through Cartesian intermediates	777

B.10.2	Recurrence relations for $E$ -coefficients	779
B.10.3	Implementation issues	780
	References	783
	Index	787