

Contents

1	Introduction	1
	References	3
2	Preliminary definitions	5
2.1	Real space vectors	5
2.2	Operators and representations	5
2.3	Simple lattices	5
2.4	“Parent” lattices	6
2.5	Reciprocal lattices	6
2.6	Brillouin zones	6
2.7	Translational groups	7
2.8	Complex lattices	8
2.9	Kohn-Sham Hamiltonians	8
2.9.1	Local spin-density functional	9
	References	9
3	Multiple scattering	11
3.1	Resolvents & Green’s functions	11
3.1.1	Basic definitions	11
3.1.2	The Dyson equation	12
3.1.3	The Lippmann-Schwinger equation	13
3.1.4	“Scaling transformations”	13
3.1.5	Integrated density of states: the Lloyd formula	14
3.2	Superposition of individual potentials	15
3.3	The multiple scattering expansion and the scattering path operator	16
3.3.1	The single-site T-operator	16
3.3.2	The multi-site T-operator	16
3.3.3	The scattering path operator	16
3.3.4	“Structural resolvents”	17
3.4	Non-relativistic angular momentum and partial wave representations	17
3.4.1	Spherical harmonics	18
3.4.2	Partial waves	18
3.4.3	Representations of $\mathcal{G}_0(z)$	19

3.4.4	Representations of the single-site \mathcal{T} -operator	22
3.4.5	Representations of $\mathcal{G}(\varepsilon)$	24
3.4.6	Representation of $\mathcal{G}(\varepsilon)$ in the basis of scattering solutions	26
3.5	Relativistic formalism	29
3.5.1	The $\kappa\mu$ -representation	29
3.5.2	The free-particle solutions	31
3.5.3	The free-particle Green's function	32
3.5.4	Relativistic single-site and multi-site scattering	38
3.6	"Scalar relativistic" formulations	41
3.7	Summary	43
	References	43
4	Shape functions	45
4.1	The construction of shape functions	45
4.1.1	Interception of a boundary plane of the polyhedron with a sphere	46
4.1.2	Semi-analytical evaluation	48
4.1.3	Shape functions for the fcc cell	49
4.2	Shape truncated potentials	52
4.2.1	Spherical symmetric potential	53
4.3	Radial mesh and integrations	54
	References	56
5	Non-relativistic single-site scattering for spherically symmetric potentials	57
5.1	Direct numerical solution of the coupled radial differential equations	57
5.1.1	Starting values	58
5.1.2	Runge-Kutta extrapolation	59
5.1.3	Predictor-corrector algorithm	60
5.2	Single site Green's function	61
5.2.1	Normalization of regular scattering solutions and the single site t matrix	62
5.2.2	Normalization of irregular scattering solutions	64
	References	64
6	Non-relativistic full potential single-site scattering	65
6.1	Schrödinger equation for a single scattering potential of arbitrary shape	65
6.2	Single site Green's function for a single scattering potential of arbitrary shape	65
6.2.1	Single spherically symmetric potential	65
6.2.2	Single potential of general shape	66

6.3	Iterative perturbational approach for the coupled radial differential equations	66
6.3.1	Regular solutions	67
6.3.2	Irregular solutions	67
6.3.3	Numerical integration scheme	68
6.3.4	Iterative procedure	69
6.4	Direct numerical solution of the coupled radial differential equations	72
6.4.1	Starting values	73
6.4.2	Runge–Kutta extrapolation	74
6.4.3	Predictor-corrector algorithm	74
6.5	Single-site t matrix	75
6.5.1	Normalization of the regular solutions	75
6.5.2	Normalization of the irregular solutions	78
	References	79
7	Spin-polarized non-relativistic single-site scattering	81
	References	82
8	Relativistic single-site scattering for spherically symmetric potentials	83
8.1	Direct numerical solution of the coupled differential equations	85
8.1.1	Starting values	85
8.1.2	Runge–Kutta extrapolation	87
8.1.3	Predictor-corrector algorithm	87
8.2	Single site Green’s function	88
8.2.1	Normalization of regular scattering solutions and the single site t matrix	89
	References	90
9	Relativistic full potential single-site scattering	91
9.1	Direct numerical solution of the coupled differential equations	91
9.1.1	Starting values	92
9.1.2	Runge–Kutta extrapolation	93
9.1.3	Predictor-corrector algorithm	94
9.1.4	Normalization of regular and irregular scattering solutions and the single-site t matrix	94
	References	94
10	Spin-polarized relativistic single-site scattering for spherically symmetric potentials	95
10.1	Direct numerical solution of the coupled radial differential equations	95

10.1.1	Evaluation of the coefficients	97
10.1.2	Coupled differential equations	98
10.1.3	Start values	99
10.1.4	Runge–Kutta extrapolation	102
10.1.5	Predictor-corrector algorithm	103
10.1.6	Normalization of the regular scattering solutions and the single site t -matrix	105
10.1.7	Normalization of the irregular scattering solutions . .	107
	References	107
11	Spin-polarized relativistic full potential single-site scattering	109
11.1	Iterative perturbational (Lippmann-Schwinger-type) approach for relativistic spin-polarized full potential single-site scattering	109
11.1.1	Redefinition of the irregular scattering solutions . . .	110
11.1.2	Regular solutions	111
11.1.3	Irregular solution	113
11.1.4	Angular momentum representations of $\Delta\mathcal{H}$	114
11.1.5	Representations of angular momenta	115
11.1.6	Calogero’s coefficients	117
11.1.7	Single-site Green’s function	119
11.2	Direct numerical solution of the coupled radial differential equations	120
11.2.1	Starting values	123
11.2.2	Runge–Kutta extrapolation	124
11.2.3	Predictor-corrector algorithm	124
11.2.4	Normalization of regular solutions	125
11.2.5	Reactance and single-site t matrix	126
11.2.6	Normalization of the irregular solution	127
	References	128
12	Scalar-relativistic single-site scattering for spherically symmetric potentials	129
12.1	Derivation of the scalar-relativistic differential equation . . .	129
12.1.1	Transformation to first order coupled differential equations	131
12.2	Numerical solution of the coupled radial differential equations	132
12.2.1	Starting values	132
	Reference	133

13	Scalar-relativistic full potential single-site scattering	135
13.1	Derivation of the scalar-relativistic differential equation	135
13.1.1	Transformation to first order coupled differential equations	137
13.2	Numerical solution of the coupled radial differential equations	138
14	Phase shifts and resonance energies	139
14.1	Non-spin-polarized approaches	139
14.2	Spin-polarized approaches	143
	References	144
15	Structure constants	145
15.1	Real space structure constants	145
15.2	Two-dimensional translational invariance	146
15.2.1	Complex “square” lattices	146
15.2.2	Multilayer systems	147
15.2.3	Real and reciprocal two-dimensional lattices	147
15.2.4	The “Kambe” structure constants	148
15.2.5	The layer- and sublattice off-diagonal case ($s \neq s'$)	149
15.2.6	The layer- and sublattice diagonal case ($s = s'$)	152
15.2.7	Simple two-dimensional lattices	153
15.2.8	Note on the “Kambe structure constants”	154
15.3	Three-dimensional translational invariance	155
15.3.1	Three-dimensional structure constants for simple lattices	155
15.3.2	Three-dimensional structure constants for complex lattices	157
15.3.3	Note on the structure constants for three-dimensional lattices	159
15.4	Relativistic structure constants	159
15.5	Structure constants and Green’s function matrix elements . .	159
	References	160
16	Green’s functions: an in-between summary	161
17	The Screened KKR method for two-dimensional translationally invariant systems	163
17.1	“Screening transformations”	163
17.2	Two-dimensional translational symmetry	165
17.3	Partitioning of configuration space	166
17.4	Numerical procedures	168
17.4.1	Inversion of block tridiagonal matrices	168
17.4.2	Evaluation of the surface scattering path operators	169
17.4.3	Practical evaluation of screened structure constants	170

17.4.4	Relativistic screened structure constants	172
17.4.5	Decaying properties of screened structure constants .	173
	References	176
18	Charge and magnetization densities	177
18.1	Calculation of physical observables	177
18.2	Non-relativistic formulation	180
18.2.1	Charge density	180
18.2.2	Charges	181
18.2.3	Partial local density of states	182
18.2.4	The spin-polarized non-relativistic case	183
18.3	Relativistic formulation	183
18.3.1	Charge density	185
18.3.2	Spin and orbital magnetization densities	186
18.3.3	Density of States	187
18.3.4	Angular momentum operators and matrix elements .	189
18.4	2D Brillouin zone integrations	190
18.5	Primitive vectors in two-dimensional lattices	191
18.6	Oblique lattice	192
18.7	Centered rectangular lattice	194
18.8	Primitive rectangular lattice	195
18.9	Square lattice	197
18.10	Hexagonal lattice	199
	References	201
19	The Poisson equation and the generalized Madelung problem for two- and three-dimensional translationally invariant systems	203
19.1	The Poisson equation: basic definitions	203
19.2	Intracell contribution	204
19.3	Multipole expansion in real-space	205
19.3.1	Charge density	205
19.3.2	Green's functions and Madelung constants	206
19.3.3	Green's functions and reduced Madelung constants .	207
19.4	Three-dimensional complex lattices	208
19.4.1	Evaluation of the Green's function for three-dimensional lattices	209
19.4.2	Derivation of Madelung constants for three- dimensional lattices	213
19.4.3	Reduced Madelung constants for three-dimensional lattices	215
19.5	Complex two-dimensional lattices	216
19.5.1	Evaluation of the Green's function for two-dimensional lattices	216

19.5.2	Derivation of the Madelung constants for two-dimensional lattices	220
19.5.3	The intercell potential	225
19.5.4	Determination of the constants \mathcal{A} and \mathcal{B}	225
19.6	A remark: density functional requirements	230
19.7	Summary	231
	References	233
20	“Near field” corrections	235
20.1	Method 1: shifting bounding spheres	235
20.2	Method 2: direct evaluation of the near field corrections ...	239
20.3	Corrections to the intercell potential	244
	References	244
21	Practical aspects of full-potential calculations	247
21.1	Influence of a constant potential shift	247
21.2	ℓ -convergence	251
	References	252
22	Total energies	253
22.1	Calculation of the total energy	253
22.2	Kinetic energy	253
22.3	Core energy	254
22.3.1	Radial Dirac equations	254
22.3.2	Numerical solution	255
22.3.3	Core charge density	256
22.3.4	Core potential	258
22.4	Band energy	259
22.4.1	Contour integration	259
22.5	Potential energy	261
22.6	Exchange and correlation energy	262
22.6.1	Numerical angular integration – Gauss quadrature ..	263
22.7	The Coulomb energy	265
22.8	A computationally efficient expression for the total energy ..	267
22.9	Illustration of total energy calculations	267
22.9.1	Computational details	269
22.9.2	Results	270
	References	273
23	The Coherent Potential Approximation	275
23.1	Configurational averages	275
23.2	Restricted ensemble averages – component projected densities of states	276
23.3	The electron self-energy operator	278
23.4	The coherent potential approximation	279

23.5	Isolated impurities	280
23.5.1	Single impurities	280
23.5.2	Double impurities	281
23.6	The single-site coherent potential approximation	282
23.6.1	Single-site CPA and restricted averages	283
23.7	The single-site CPA equations for three-dimensional translational invariant systems	284
23.7.1	Simple lattices	284
23.7.2	Complex lattices	285
23.8	The single-site CPA equations for two-dimensional translational invariant systems	287
23.8.1	Simple parent lattices	287
23.8.2	Complex lattices	289
23.9	Numerical solution of the CPA equations	290
	References	291
24	The embedded cluster method	293
24.1	The Dyson equation of embedding	293
24.2	An embedding procedure for the Poisson equation	294
24.3	Convergence with respect to the size of the embedded cluster	298
	References	298
25	Magnetic configurations – rotations of frame	299
25.1	Rotational properties of the Kohn-Sham-Dirac Hamiltonian	299
25.2	Translational properties of the Kohn-Sham Hamiltonian	301
25.3	Magnetic ordering and symmetry	302
25.3.1	Translational restrictions	302
25.3.2	Rotational restrictions	302
25.4	Magnetic configurations	303
25.4.1	Two-dimensional translational invariance	303
25.4.2	Complex lattices	303
25.4.3	Absence of translational invariance	304
25.5	Rotation of frames	304
25.5.1	Rotational properties of two-dimensional structure constants	305
25.6	Rotational properties and Brillouin zone integrations	307
	References	309
26	Related physical properties	311
26.1	Surface properties	311
26.1.1	Potentials at surfaces	312
26.1.2	Work function	316
26.2	Applications of the fully relativistic spin-polarized Screened KKR-ASA scheme	317

26.3	Interlayer exchange coupling, magnetic anisotropies, perpendicular magnetism and reorientation transitions in magnetic multilayer systems	317
26.3.1	Energy difference between different magnetic configurations	317
26.3.2	Interlayer exchange coupling (IEC)	319
26.3.3	An example: the Fe/Cr/Fe system	319
26.3.4	Magnetic anisotropy energy (E_a)	320
26.3.5	Disordered systems	323
26.3.6	An example: $Ni_n/Cu(100)$ and $Co_m/Ni_n/Cu(100)$..	324
26.4	Magnetic nanostructures	326
26.4.1	Exchange energies, anisotropy energies	326
26.4.2	An example Co clusters on Pt(100)	330
26.5	Electric transport in semi-infinite systems	337
26.5.1	Bulk systems	337
26.5.2	An example: the anisotropic magnetoresistance (AMR) in permalloy ($Ni_{1-c}Fe_c$)	339
26.5.3	Spin valves: the giant magneto-resistance	340
26.5.4	An example: the giant magneto-resistance in Fe/Au/Fe multilayers	342
26.6	Magneto-optical transport in semi-infinite systems	347
26.6.1	The (magneto-) optical tensor	347
26.6.2	An example: the magneto-optical conductivity tensor for Co on Pt(111)	348
26.6.3	Kerr angles and ellipticities	349
26.6.4	An example: the optical constants in the “bulk” systems Pt(100), Pt(110), Pt(111)	354
26.7	Mesoscopic systems: magnetic domain walls	354
26.7.1	Phenomenological description of domain walls	354
26.7.2	Ab initio domain wall formation energies	357
26.7.3	An example: domain walls in bcc Fe and hcp Co ...	358
26.7.4	Another example: domain wall formation in permalloy	359
26.7.5	Domain wall resistivities	361
26.7.6	An example: the CIP-AMR in permalloy domain walls	365
26.8	Spin waves in magnetic multilayer systems	365
26.8.1	An example: magnon spectra for magnetic monolayers on noble metal substrates	370
	References	372
A	Appendix: Useful relations, expansions, functions and integrals	375
	References	379

<http://www.springer.com/978-3-540-22524-9>

Electron Scattering in Solid Matter

A Theoretical and Computational Treatise

Zabloudil, J.; Hammerling, R.; Szunyogh, L.; Weinberger,

P.

2005, XVI, 382 p., Hardcover

ISBN: 978-3-540-22524-9