Elementary Scattering Theory

For X-ray and neutron users

D.S. SIVIA

St John's College, Oxford

Contents

I	Some preliminaries	1
1	Studying matter at the atomic and molecular level	3
1.1	Length scales and logarithmic axes	3
1.2	Resolution, magnification and microscopy	6
1.3	Structure, dynamics and spectroscopy	9
1.4	Atomic building blocks and interactions	11
1.4.1	The basic structure of the atom	12
1.4.2	The fundamental forces of nature	13
1.4.3	Probing matter by scattering particles	14
1.5	Energy, length and temperature scales	16
1.6	A table of useful constants	18
2	Waves, complex numbers and Fourier transforms	19
2.1	Sinusoidal waves	19
2.1.1	The direction of propagation	21
2.1.2	The principle of superposition	23
2.2	Complex numbers	25
2.2.1	Definition	25
2.2.2	Basic algebra	26
2.2.3	The Argand diagram	27
2.2.4	The imaginary exponential	27
2.3	Fourier series	29
2.3.1	Orthogonality and the Fourier coefficients	30
2.3.2	The complex Fourier series	32
2.4	Fourier transforms	32
2.4.1	Convolution theorem	34
2.4.2	Auto-correlation function	36
2.5	Fourier optics and physical insight	38
2.5.1	Young's double slit	40
2.5.2	A single wide slit	41
2.5.3	A diffraction grating	42
2.5.4	The convolution theorem in action	43
2.5.5	Multi-dimensional generalization	44
2.6	Fourier data analysis	48
2.6.1	The phase problem	48
2.6.2	Truncation effects and windowing	50
2.6.3	Noise and probability theory	52

2.7	A list of useful formulae	56
2.7.1	Dimensional analysis	59
II	Elastic scattering	61
3	The basics of X-ray and neutron scattering	63
3.1	An idealized scattering experiment	63
3.1.1	Elastic scattering and momentum transfer	64
3.1.2	The differential cross-section	66
3.1.3	Elastic versus total scattering	67
3.2	Scattering by a single fixed atom	67
3.2.1	Nuclear scattering lengths	69
3.2.2	Atomic form factors	71
3.2.3	Magnetic form factors	73
3.2.4	Scattering cross-sections	75
3.3	Scattering from an assembly of atoms	77
3.3.1	Scattering density and Fourier transforms	79
3.3.2	Temperature and Debye—Waller factors	81
3.3.3	Coherent and incoherent scattering	82
3.3.4	Mixed scattering events	84
3.4	X-rays and synchrotron sources	84
3.4.1	Wigglers and undulators	88
3.5	Reactors and pulsed neutron sources	89
3.5.1	The time-of-flight technique	91
4	Surfaces, interfaces and reflectivity	93
4.1	Reflectivity and Fourier transforms	93
4.1.1	Substrate only	98
4.1.2	One uniform layer	100
4.1.3	A short multilayer	101
4.1.4	A phaseless Fourier ambiguity	102
4.2	Reflectivity and geometrical optics	104
4.2.1	Refractive index	105
4.2.2	A single boundary	105
4.2.3	Multiple boundaries	108
4.3	X-rays, neutrons and other techniques	110
5	Small-angle scattering and the big picture	113
5.1	Diffraction and length scales	113
5.2	Size, shape and molecular form factors	114
5.2.1	Absolute intensities	118
5.2.2	The Guinier approximation	119
5.2.3	Porod's law	122
5.2.4	Polydispersity	124
5.3	Assemblies and correlations	125
5.3.1	Orientational alignment	125
5.3.2	Positional correlation	126
5.4	Pair-distribution function	127

5.5	Contrast matching	129
6	Liquids and amorphous materials	131
6.1	The middle phase of matter	131
6.2	Radial distribution functions	132
6.3	Structure factors	134
6.3.1	Partial structure factors	137
6.4	Comparison with small-angle scattering	139
6.5	The Placzek correction	139
7	Periodicity, symmetry and crystallography	141
7.1	Repetitive structures and Bragg peaks	141
7.1.1	Atomic planes and Bragg's law	144
7.1.2	Simple consequences and applications	146
7.2	Patterns and symmetries	147
7.2.1	Reality and Friedel pairs	147
7.2.2	Centrosymmetry and reality	148
7.2.3	Space groups and systematic absences	148
7.2.4	Geometry and space groups	150
7.2.5	Symmetry and statistics	151
7.3	Circumventing the phase problem	151
7.3.1	Patterson maps	152
7.3.2	Heavy atoms and partial structure	153
7.3.3	Isomorphous replacement	154
7.3.4	Direct methods and prior knowledge	155
7.4	Powdered samples	156
7.4.1	Texture	158
7.4.2	Twinning	159
7.4.3	Fibre diffraction	160
7.5	Magnetic structures	160
III	Inelastic scattering	163
8	Energy exchange and dynamical information	165
8.1	Experimental considerations	165
8.1.1	The partial differential cross-section	166
8.1.2	Triple-axis spectrometer	167
8.1.3	Time-of-flight instruments	168
8.2	Scattering from time-varying structures	169
8.2.1	Elastic scattering	170
8.2.2	Space—time correlation function	170
8.2.3	Total scattering	171
8.2.4	Coherent and incoherent scattering	172
8.3	A quantum transitions approach	173
9	Examples of inelastic scattering	175
9.1	Compton scattering	175
9.1.1	The impulse approximation	177

9.1.2	Single particle wave function	178
9.2	Lattice vibrations	179
9.2.1	Heat capacities	182
9.2.2	Spin waves	183
9.3	Molecular spectroscopy	184
9.3.1	Quasi-elastic scattering	185
9.3.2	Energy resolution and time-scales	186
<hr/>		
A Discrete Fourier transforms		187
<hr/>		
B Resonant scattering and absorption		191
<hr/>		
References		193
Index		197