

Contents

Part I Basic Concepts in Frustrated Magnetism

1 Geometrically Frustrated Antiferromagnets: Statistical Mechanics and Dynamics	3
John T. Chalker	
1.1 Introduction	3
1.2 Models	5
1.3 Some Experimental Facts	6
1.4 Classical Ground State Degeneracy	8
1.5 Order by Disorder	10
1.6 Ground State Correlations	14
1.7 Dynamics	17
1.8 Final Remarks	21
References	21
2 Introduction to Quantum Spin Liquids	23
Claire Lhuillier and Grégoire Misguich	
2.1 Introduction	23
2.2 Basic Building Blocks of VBC and RVB Physics: The Valence Bonds	27
2.3 Valence-Bond Crystals	29
2.3.1 Zeroth-Order VBC Wave Function	30
2.3.2 Quantum Fluctuations in VBCs	31
2.3.3 VBC Excitations	32
2.4 Resonating-Valence-Bond Spin Liquids	33
2.5 VBCs or RVB Spin Liquids on Kagomé and Pyrochlore Lattices?	36
2.6 Conclusion	38
References	39

Part II Probing Frustrated Magnets

3 Neutron Scattering and Highly Frustrated Magnetism	45
Steven T. Bramwell	
3.1 Introduction	45
3.2 What Neutron Scattering Measures	47
3.2.1 Scattering Triangle	47
3.2.2 Partial Differential Cross Section	48
3.2.3 Relation to Sample Properties	49
3.2.4 Scattering from Atomic Magnetic Moments	50
3.2.5 Orientation Factor and Form Factor	50
3.2.6 General Expression for the Neutron Scattering	51
3.2.7 Real Experiments	52
3.2.8 Powder Averaging	52
3.2.9 Static Approximation	52
3.2.10 Wavevector Dependent Magnetic Moment and Susceptibility	53
3.2.11 Fully Ordered Magnet	54
3.2.12 Magnet with Full or Partial Disorder	55
3.2.13 Validity of the Static Approximation	55
3.2.14 Generalised Susceptibility	56
3.2.15 Neutron Spectroscopy	57
3.3 Typical Neutron Scattering Patterns	58
3.3.1 Scattering Plane	58
3.3.2 Free Energy	58
3.3.3 Ideal Paramagnet	60
3.3.4 Conventional Magnet Above T_C	60
3.3.5 Conventional Magnet Below T_C	61
3.3.6 Cooperative Paramagnet	62
3.3.7 Absent Pinch Points	63
3.3.8 Dynamical Signature of Cooperative Paramagnetism	64
3.4 Experimental Results	65
3.4.1 Cooperative Paramagnet States	65
3.4.2 Ordered States	70
3.4.3 Excited States	74
3.5 Conclusions	76
References	77
4 NMR and μSR in Highly Frustrated Magnets	79
Pietro Carretta and Amit Keren	
4.1 Basic Aspects of NMR and μ SR Techniques	79
4.1.1 Line Shift and Line Width	80
4.1.2 Nuclear and Muon Spin-Lattice Relaxation Rate $1/T_1$	83
4.1.3 μ SR: The Static Case	85
4.1.4 μ SR: The Dynamic Case	88

4.2	From Zero- to Three-Dimensional Frustrated Magnets	91
4.2.1	Molecular Magnets	91
4.2.2	Antiferromagnets on a Square Lattice with Competing Interactions: The J_1 - J_2 Model	92
4.2.3	Magnetic Frustration on a Triangular Lattice.....	95
4.2.4	μ SR and NMR in the Spin-1/2 Kagomé Lattice $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$	97
4.2.5	The Problem of μ^+ Relaxation in Some Kagomé Lattices	98
4.2.6	Persistent Dynamics and Lattice Distortions in the Pyrochlore Lattice	101
	References	103
5	Optical Techniques for Systems with Competing Interactions	107
	Joachim Deisenhofer and Peter Lemmens	
5.1	Introduction	107
5.2	Inelastic Light-Scattering	108
5.3	Inelastic Phonon Light-Scattering.....	110
5.4	Inelastic Magnetic, Quasielastic, and Electronic Light Scattering	111
5.5	The IR Experiment.....	115
5.6	Spins, Phonons, and Light	116
5.7	Spin–Phonon Interaction in Cr Spinels	118
5.8	Exciton–Magnon Absorption in KCuF_3	122
	References	124
Part III Frustrated Systems		
6	The Geometries of Triangular Magnetic Lattices	131
	Robert J. Cava, Katharine L. Holman, Tyrel McQueen, Eric J. Welsh, D. Vincent West, and Anthony J. Williams	
6.1	Introduction	131
6.2	Two-Dimensional Structures	132
6.2.1	Planes of Edge-Sharing Triangles.....	132
6.2.2	Planes of Corner-Sharing Triangles.....	136
6.3	Three-Dimensional Structures.....	141
6.4	Note on Synthesis of the Compounds	151
6.5	Conclusion	151
	References	152
7	Highly Frustrated Magnetism in Spinels	155
	Hidenori Takagi and Seiji Niitaka	
7.1	Introduction	155
7.2	Spinel Structure	156
7.3	Basic Electronic Configuration.....	157

7.4	Uniqueness of the Spinel as a Frustrated Magnet	157
7.5	Materials Overview of Spinels	159
7.6	Frustration in Selected Spinels	161
7.6.1	Pyrochlore Antiferromagnets in Spinel Oxides – B-site Frustration	161
7.6.2	Frustrated Spins on Spinel A Sites	167
7.6.3	Frustrated Magnets based on Cation- ordered Spinels: The Hyper-Kagomé Lattice of $\text{Na}_4\text{Ir}_3\text{O}_8$	168
7.6.4	Charge Frustration in Mixed-valent Spinels	171
7.7	Summary	172
	References	173
8	Experimental Studies of Pyrochlore Antiferromagnets	177
	Bruce D. Gaulin and Jason S. Gardner	
8.1	Introduction	177
8.2	The Cubic Pyrochlores	178
8.3	The Spin Liquid Ground State in $\text{Tb}_2\text{Ti}_2\text{O}_7$	180
8.4	Ordered Ground States in $\text{Tb}_2\text{Ti}_2\text{O}_7$	185
8.5	Structural Fluctuations in the Spin Liquid State of $\text{Tb}_2\text{Ti}_2\text{O}_7$	190
8.6	Magnetic Order and Fluctuations in $\text{Tb}_2\text{Sn}_2\text{O}_7$	195
8.6.1	Phase Transitions and Fluctuations in $\text{Gd}_2\text{Ti}_2\text{O}_7$ and $\text{Gd}_2\text{Sn}_2\text{O}_7$	198
8.7	Conclusions	203
	References	204
9	Kagomé Antiferromagnets: Materials Vs. Spin Liquid Behaviors	207
	Philippe Mendels and Andrew S. Wills	
9.1	A Short Theoretical Survey: What would be the Ideal Kagomé Antiferromagnet?	208
9.2	The Jarosites	210
9.2.1	Synthesis and the Jarosite Crystal Structure: Idealized and Disordered	210
9.2.2	Fe jarosites: $S = \frac{5}{2}$ Kagomé Antiferromagnets	215
9.2.3	Cr Jarosites- $S = \frac{3}{2}$ Kagomé Antiferromagnets	217
9.2.4	Conclusion	218
9.3	Pyrochlore Slabs	218
9.3.1	Synthesis	218
9.3.2	Magnetic Network	219
9.3.3	Generic Physics	220
9.3.4	Non-magnetic Defects	222
9.3.5	Concluding Remarks	224
9.4	Towards $S = 1/2$ Ideal Compounds	225
9.4.1	Volborthite	225

9.4.2	Herbertsmithite: “An end to the Drought of Quantum Spin Liquids [100]”.....	228
9.5	Other Compounds.....	233
9.5.1	Organic Materials	233
9.5.2	$Y_{0.5}Ca_{0.5}BaCo_4O_7$	234
9.5.3	Langasites	234
9.6	Conclusion	235
	References.....	236

Part IV Specific Effects in Frustrated Magnets

10	Magnetization Plateaus	241
	Masashi Takigawa and Frédéric Mila	
10.1	Introduction	241
10.2	Mechanisms for Formation of Magnetization Plateaus	242
10.2.1	Spin Gap	243
10.2.2	Quantized Plateaus.....	244
10.2.3	Order by Disorder.....	245
10.2.4	Superfluid-Insulator Transition.....	246
10.2.5	‘Quantum’ Plateaus	247
10.2.6	High-Order Plateaus	249
10.2.7	Transition into Plateaus.....	250
10.3	Experimental Observation of Magnetization Plateaus	251
10.3.1	‘Classical’ Plateaus in Triangular and Pyrochlore Lattices	252
10.3.2	$SrCu_2(BO_3)_2$ and the Shastry–Sutherland Model.....	255
10.3.3	‘Quantum’ Plateaux and Spin Superstructure in $SrCu_2(BO_3)_2$	258
10.3.4	Phase Diagram of $SrCu_2(BO_3)_2$	261
10.3.5	RB_4 : A New Family of Shastry–Sutherland System.....	263
10.4	Conclusion	264
	References.....	264
11	Spin-Lattice Coupling in Frustrated Antiferromagnets.....	269
	Oleg Tchernyshov and Gia-Wei Chern	
11.1	Introduction	269
11.2	Spin-Driven Jahn–Teller Effect in a Tetrahedron.....	270
11.2.1	Generalized Coordinates and Forces	271
11.2.2	Four $S = 1/2$ Spins on a Tetrahedron	273
11.2.3	Four Classical Spins on a Tetrahedron.....	275
11.2.4	Color Notation and Other Useful Analogies.....	276
11.2.5	Spin–Jahn–Teller Effect on a Triangle	276
11.3	Models with Local Phonon Modes	278
11.3.1	Half-Magnetization Plateau in ACr_2O_4 Spinel	279

11.4	Collective Spin–Jahn–Teller Effect on the Pyrochlore Lattice	280
11.5	Collective Jahn–Teller Effect in CdCr_2O_4	282
11.5.1	Spiral Magnetic Order in CdCr_2O_4	283
11.5.2	Theory of Spiral Magnetic Order	284
11.6	Summary and Open Questions	289
	References	290
12	Spin Ice	293
	Michel J.P. Gingras	
12.1	Introduction	293
12.2	Water Ice, Pauling Entropy, and Anderson Model	294
12.2.1	Water Ice and Pauling Model	294
12.2.2	Cation Ordering in Inverse Spinels and Antiferromagnetic Pyrochlore Ising Model	296
12.3	Discovery of Spin Ice	298
12.3.1	Rare-Earth Pyrochlore Oxides: Generalities	298
12.3.2	Microscopic Hamiltonian: Towards an Effective Ising Model	299
12.3.3	Discovery of Spin Ice in $\text{Ho}_2\text{Ti}_2\text{O}_7$	304
12.3.4	Nearest-Neighbor Ferromagnetic $\langle 111 \rangle$ Ising Model and Pauling’s Entropy	305
12.3.5	Residual Entropy of $\text{Dy}_2\text{Ti}_2\text{O}_7$ and $\text{Ho}_2\text{Ti}_2\text{O}_7$	307
12.4	Dipolar Spin-Ice Model	309
12.4.1	Competing Interactions in the Dipolar Spin-Ice Model	309
12.4.2	Mean-Field Theory	312
12.4.3	Loop Monte Carlo Simulations and Phase Diagram of Dipolar Spin Ice	316
12.4.4	Origin of Ice Rules in Dipolar Spin Ice	318
12.5	Current Research Topics in Spin Ices and Related Materials	319
12.5.1	Magnetic-Field Effects	319
12.5.2	Dynamical Properties and Role of Disorder	322
12.5.3	Beyond the Dipolar Spin-Ice Model	322
12.5.4	Metallic Spin Ice	322
12.5.5	Artificial Spin Ice	323
12.5.6	Stuffed Spin Ice	323
12.5.7	Quantum Mechanics, Dynamics, and Order in Spin Ices	323
12.5.8	Coulomb Phase, Monopoles and Dirac Strings in Spin Ices	324
12.6	Conclusion	325
	References	326

13 Spin Nematic Phases in Quantum Spin Systems	331
Karlo Penc and Andreas M. Läuchli	
13.1 Introduction and Materials	331
13.2 Multipolar States of a Single Spin	333
13.3 Competition Between Dipoles and Quadrupoles	336
13.3.1 The Bilinear–Biquadratic Model	336
13.3.2 Energy Spectra of Small Clusters	338
13.4 Quadrupolar Ordering in $S = 1$ Systems.....	340
13.4.1 Variational Phase Diagram	340
13.4.2 One- and Two-Magnon Instability of the Fully Polarized State	346
13.4.3 Spin-Wave Theory for the Ferroquadrupolar Phase ..	347
13.4.4 Numerical Approach.....	353
13.5 From Chains to the Square Lattice	355
13.6 Nematic Ordering in $S = 1/2$ Systems	357
13.7 Conclusions	359
References.....	360

Part V Advanced Theoretical Methods and Concepts in Frustrated Magnetism

14 Schwinger Bosons Approaches to Quantum Antiferromagnetism	365
Assa Auerbach and Daniel P. Arovas	
14.1 $SU(N)$ Heisenberg Models	365
14.2 Schwinger Representation of $SU(N)$ Antiferromagnets	366
14.2.1 Bipartite Antiferromagnet	367
14.2.2 Non-bipartite (Frustrated) Antiferromagnets	368
14.3 Mean Field Hamiltonian	369
14.3.1 Mean Field Equations	371
14.4 The Mean Field Antiferromagnetic Ground State	373
14.5 Staggered Magnetization in the Layered Antiferromagnet	375
References.....	377

15 Variational Wave Functions for Frustrated Magnetic Models	379
Federico Becca, Luca Capriotti, Alberto Parola, and Sandro Sorella	
15.1 Introduction	379
15.2 Symmetries of the Wave Function: General Properties	382
15.3 Symmetries in the Two-dimensional Case	384
15.3.1 The Marshall–Peierls Sign Rule	386
15.3.2 Spin Correlations	387
15.4 Connection with the Bosonic Representation	388
15.5 Antiferromagnetic Order	390

15.6	Numerical Results	392
15.6.1	One-dimensional Lattice	392
15.6.2	Two-dimensional Lattice	396
15.7	Other Frustrated Lattices	402
15.8	Conclusions	404
	References	405
16	Quantum Spin Liquids and Fractionalization	407
	Grégoire Misguich	
16.1	Introduction	407
16.2	What is a Spin Liquid?	409
16.2.1	Absence of Magnetic Long-Range Order (Definition 1)	409
16.2.2	Absence of Spontaneously Broken Symmetry (Definition 2)	409
16.2.3	Fractional Excitations (Definition 3).....	410
16.2.4	Half-odd-integer Spins and the Lieb-Schultz-Mattis-Hastings Theorem	415
16.3	Mean Fields and Gauge Fields	416
16.3.1	Fermionic Representation of Heisenberg Models	416
16.3.2	Local $SU(2)$ Gauge Invariance	418
16.3.3	Mean-field (Spin-liquid) States	418
16.3.4	Gauge Fluctuations	422
16.4	\mathbb{Z}_2 Spin Liquids	427
16.4.1	Short-range RVB Description	427
16.4.2	\mathbb{Z}_2 Gauge Theory, Spinon Deconfinement, and Vasons	428
16.4.3	Examples	430
16.4.4	How to Detect a Gapped \mathbb{Z}_2 Liquid.....	431
16.5	Gapless (Algebraic) Liquids.....	432
16.6	Other Spin Liquids.....	432
16.7	Conclusion	433
	References	433
17	Quantum Dimer Models	437
	Roderich Moessner and Kumar S. Raman	
17.1	Introduction	437
17.2	How Quantum Dimer Models Arise	438
17.2.1	Link Variables and Hard Constraints	438
17.2.2	The Origin of Constraints	439
17.2.3	Tunable Constraints.....	440
17.2.4	Adding Quantum Dynamics.....	441
17.3	The Quantum Dimer Model Hilbert Space	443
17.3.1	Topological Invariants	443
17.3.2	Topological Order.....	445
17.3.3	Fractionalisation	446

17.4	QDM Phase Diagrams	447
17.4.1	General Structure of Phase Diagrams.....	447
17.4.2	Z_2 RVB Liquid Phase	449
17.4.3	U(1) RVB Liquid Phase	451
17.4.4	Deconfined Critical Points.....	452
17.4.5	Valence Bond Crystals.....	452
17.4.6	Summary of Phase Diagrams.....	455
17.5	The Rokhsar–Kivelson Point	456
17.5.1	Ground-state Wavefunction	456
17.5.2	Fractionalisation and Deconfinement.....	457
17.5.3	Spatial Correlations	457
17.5.4	Excited States	458
17.5.5	A Special Liquid Point or part of a Liquid Phase?	459
17.6	Resonons, Photons, and Pions: Excitations in the Single mode Approximation	460
17.7	Dualities and Gauge Theories	462
17.7.1	Emergence of the QDM	463
17.7.2	Continuum Limit of the Gauge Theory	464
17.8	Height Representation	465
17.9	Numerical Methods	470
17.10	Dimer Phases in SU(2) Invariant Models	471
17.10.1	Overlap Expansion	472
17.10.2	Decoration.....	473
17.10.3	Large-N.....	474
17.10.4	Klein Models: SU(2) Invariant Spin Liquids	475
17.11	Outlook	475
17.11.1	Hopping Fermions	476
17.11.2	... and much more	476
	References.....	477
18	Numerical Simulations of Frustrated Systems	481
	Andreas M. Läuchli	
18.1	Overview of Methods	481
18.2	Classical Monte Carlo	481
18.3	Quantum Monte Carlo	485
18.3.1	Stochastic Series Expansion (SSE)	485
18.3.2	Green-function Monte Carlo	487
18.4	Series Expansions	488
18.4.1	High-temperature Series	488
18.4.2	$T = 0$ Perturbative Expansions for Ground- and Excited-state Properties	489
18.5	Density-Matrix Renormalization Group (DMRG)	489
18.5.1	Finite T	490
18.5.2	Dynamical Response Functions	490
18.5.3	DMRG in two and more Dimensions	491

18.6	Exact Diagonalization (ED)	491
18.6.1	Basis Construction	492
18.6.2	Coding of Basis States	493
18.6.3	Symmetrized Basis States	494
18.6.4	Hamiltonian	496
18.6.5	Eigensolvers	497
18.6.6	Implementation Details and Performance Aspects	499
18.6.7	Observables	500
18.6.8	Dynamical Response Functions	503
18.6.9	Time Evolution	504
18.6.10	Finite Temperatures	505
18.7	Miscellaneous Further Methods	506
18.7.1	Classical Spin Dynamics (Molecular Dynamics)	506
18.7.2	Coupled-Cluster Method	506
18.7.3	Dynamical Mean-Field Theory (DMFT)	507
18.7.4	Contractor Renormalization (CORE)	507
18.7.5	SR-RVB Calculations	507
18.8	Source Code Availability	508
	References	509
19	Exact Results in Frustrated Quantum Magnetism	513
	Shin Miyahara	
19.1	Introduction	513
19.1.1	Dimer Model	514
19.2	Exact Results in Spin-1/2 Heisenberg Models	515
19.2.1	Exact Ground States in Coupled Triangular Cluster Models	516
19.2.2	Exact Ground States in Coupled Tetrahedral Cluster Models	522
19.2.3	Realization of Exact Ground States	524
19.3	Exact Results in Frustrated Spin-1/2 Models with Four-Spin Interactions	526
19.3.1	General Ladder Model with Four-Spin Interactions	526
19.3.2	Two-Dimensional Model with Four-Spin Interactions	531
19.4	Conclusion	534
	References	535
20	Strong-Coupling Expansion and Effective Hamiltonians	537
	Frédéric Mila and Kai Phillip Schmidt	
20.1	Introduction	537
20.2	Strong-Coupling Expansion	538
20.2.1	Second-Order Perturbation Theory	539
20.2.2	High-Order Perturbation Theory	539
20.2.3	Examples	540

20.3	Alternative Approaches Yielding Effective Hamiltonians	547
20.3.1	Canonical Transformation	547
20.3.2	Continuous Unitary Transformation	548
20.3.3	Contractor Renormalization	555
20.4	Conclusions	556
	References	558

Part VI Frustration, Charge Carriers and Orbital Degeneracy

21	Mobile Holes in Frustrated Quantum Magnets and Itinerant Fermions on Frustrated Geometries	563
	Didier Poilblanc and Hirokazu Tsunetsugu	
21.1	Introduction	563
21.2	Doping Holes in Frustrated Quantum Magnets.....	564
21.2.1	The Holon–Spinon Deconfinement Scenario	564
21.2.2	Single Hole Doped in Frustrated Mott Insulators	565
21.2.3	Hole Pairing and Superconductivity	568
21.3	Doped Quantum Dimer Model	569
21.3.1	Origin of the Quantum Dimer Model	569
21.3.2	Phase Diagrams at Zero Doping	571
21.3.3	Connection to the XXZ Magnet on the Checkerboard Lattice	571
21.3.4	Bosonic Doped Quantum Dimer Model	573
21.3.5	Non-Frobenius Doped Quantum Dimer Model on the Square Lattice	574
21.4	Mott Transition on the Triangular Lattice	575
21.4.1	Frustration in Itinerant Electron Systems	575
21.4.2	Mott Transition in Organic Compounds with Triangular Geometry	575
21.4.3	Mott Transition in the Triangular-Lattice Hubbard Model	576
21.5	Ordering Phenomena at Commensurate Fermion Densities on Frustrated Geometries	579
21.5.1	Bond Order Waves from Nesting Properties of the Fermi surface.....	580
21.5.2	Metal–Insulator Transitions and Frustrated Charge Order	581
21.5.3	Away from Commensurability: Doping the Resonating-Singlet-Pair Crystal.....	583
21.6	Summary	584
	References	584

22 Metallic and Superconducting Materials with Frustrated Lattices.....	587
Zenji Hiroi and Masao Ogata	
22.1 Introduction	587
22.2 Materials Overview	590
22.2.1 Pyrochlore Lattice	590
22.2.2 Triangular and Kagomé Lattices	596
22.2.3 Organic Conductors with Triangular Lattice	599
22.3 Theoretical Background	604
22.3.1 RVB Spin State and RVB Superconductivity.....	604
22.3.2 Triangular-Lattice Hubbard Model	607
22.3.3 Extended Hubbard Model for Organic Conductors	609
22.4 Superconducting Compounds	611
22.4.1 Pyrochlore Lattice: $Cd_2Re_2O_7$ and AOs_2O_6	611
22.4.2 Triangular Lattice: Na_xCoO_2 and Its Hydrate.....	616
22.4.3 Anisotropic Triangular Lattice: Organic Superconductivity.....	620
22.5 Summary	621
References.....	621
23 Frustration in Systems with Orbital Degrees of Freedom	629
Jeroen van den Brink, Zohar Nussinov, and Andrzej M. Oleś	
23.1 Introduction	629
23.2 Orbital Degrees of Freedom	630
23.2.1 Orbitals and Their Energy Scales	630
23.2.2 Comparing Orbital and Spin Degrees of Freedom	632
23.3 Orbital Interactions and Orbital Models	634
23.3.1 Crystal-Field Splitting of Orbitals	634
23.3.2 Jahn-Teller Deformation	634
23.3.3 Jahn-Teller-Mediated Orbital–Orbital Interactions	636
23.3.4 Superexchange-Mediated Orbital–Orbital Interactions	638
23.4 Symmetry and Symmetry-Breaking in Orbital Models	638
23.4.1 Types of Symmetry in Orbital Models.....	638
23.4.2 Examples of Intermediate Symmetries in Orbital Systems	639
23.4.3 A Theorem on Dimensional Reduction	642
23.4.4 Consequences of the Theorem for Orbital (and Spin) Orders and Excitations	645
23.5 Order by Disorder in Classical Orbital Models.....	646
23.6 Connection with Quantum Computation	649
23.6.1 Kitaev’s Honeycomb Model.....	649
23.6.2 Kitaev’s Toric Code model	651
23.6.3 Recent Discussions of Quantum Computing Realizations	652

23.7	Spin-Orbital Frustration	652
23.7.1	General Structure of Spin-Orbital Superexchange Models	652
23.7.2	Spin-Orbital Models for e_g Perovskites	653
23.7.3	Spin-Orbital Superexchange for t_{2g} Perovskites	657
23.7.4	Spin-Orbital Frustration on a Triangular Lattice	661
23.7.5	Spin-Orbital Frustration in Spinels	664
23.8	Spin-Orbital Entanglement	665
	References.....	668
	Index.....	671