Contents

1	Inti	roduction	1
	1.1	Spin-charge Coupled Systems	1
	1.2	Magnetism in Spin-Charge Coupled Systems	3
		1.2.1 Ruderman-Kittel-Kasuya-Yosida Interaction	3
		1.2.2 Double-Exchange Interaction	5
		1.2.3 Magnetic Ordering by a Metal-Insulator Transition	7
	1.3	Transport Phenomena in Spin-Charge Coupled Systems	8
		1.3.1 Metal-Insulator Transition	8
		1.3.2 Electron Scattering by Localized Moments	8
		1.3.3 Anomalous Hall Effect Induced by the Spin Berry Phase	9
	1.4	Pyrochlore Oxides	10
		1.4.1 Lattice and Electronic Structure	11
		1.4.2 Geometrical Frustration in Pyrochlore Magnets	12
		1.4.3 Subdominant Interactions in Spin Ice Compounds	14
		1.4.4 Metallic Pyrochlore Magnets	14
		1.4.5 $R_2 Mo_2 O_7$	15
		1.4.6 $R_2 \operatorname{Ir}_2 \operatorname{O}_7$	20
	1.5	Triangular Layered Oxides	23
		1.5.1 Partially Disordered State	23
		1.5.2 Ag_2CrO_2	25
	1.6	Motivation of This Study	26
	1.7	Structure of This Thesis	27
2	Mo	odels and Methods	29
	2.1	Ising-Spin Kondo Lattice Model	29
		2.1.1 Kondo Lattice Model on Frustrated Lattices	29
		2.1.2 Strong Coupling Limit	30
	2.2	Monte Carlo Simulation	30
	2.3	Polynomial Expansion Method	31
		2.3.1 Truncation Algorithm	32
		2.3.2 Physical Quantities	33
		2.3.3 Conductivity	34

	2.4	Variational Method	35
	2.5	Perturbation Method in the Strong Coupling Limit	35
3	Par	tial Disorder on a Triangular Lattice	39
	3.1	Model and Method	39
		3.1.1 Model	39
		3.1.2 Physical Quantities	40
	3.2	Mean Field Theory	43
	3.3	Monte Carlo Simulation	46
		3.3.1 Phase Diagrams	46
		3.3.2 Partial Disorder	49
		3.3.3 Other Magnetic Orders	52
		3.3.4 Phase Separation	57
	3.4	Electronic State	58
	3.5	Summary	60
4	Dira	ac Half-Metal on a Triangular Lattice	61
	4.1	Model and Method	61
		4.1.1 Model	61
		4.1.2 Numerical Calculations	61
	4.2	Dirac Nodes in Honeycomb and Kagome Lattices	63
	4.3	Band Structure	63
	4.4	Low-Energy Effective Hamiltonian	66
		4.4.1 $\mathbf{k} \cdot \mathbf{p}$ Perturbation Theory	66
		4.4.2 Condition for the Dirac Half-Metal	67
	4.5	Phase Diagrams	68
	4.6	Discussion and Summary	70
5	The	ermally-Induced Phases on a Kagome Lattice	73
	5.1	Model and Method	73
		5.1.1 Model	73
		5.1.2 Monte Carlo Method	74
		5.1.3 Variational Calculation	74
		5.1.4 Observables \ldots	74
	5.2	Loop-Liquid State	76
		5.2.1 Phase Diagram	76
		5.2.2 Loop Liquid and Its Crystalization	79
		5.2.3 Resonant Peak in the Electronic State	80
	5.3	Partial Disorder	83
	5.4	Summary	85
		v	

6	And	omalous Hall Insulator in Kagome Ice	87
	6.1	Model and Method	87
		6.1.1 Kagome Ice Model	87
		6.1.2 Numerical Diagonalization	89
		6.1.3 Monte Carlo Simulation	89
	6.2	Exact Diagonalization Study of Electronic States	90
		6.2.1 Density of States	90
		6.2.2 In-Gap Localized States	91
		6.2.3 Conductivity	91
	6.3	Monte Carlo Simulation	94
		6.3.1 Magnetic Properties	94
		6.3.2 Electronic and Transport Properties	96
	6.4	Anisotropic Pyrochlore Lattice	97
	6.5	Discussions and Summary	99
7	Spi	n-charge Coupled Phases on a Pyrochlore Lattice	101
	7.1	Model and Method	101
		7.1.1 Spin-Ice Kondo Lattice Model	101
		7.1.2 Monte Carlo Simulation	102
		7.1.3 Physical Quantities	102
	7.2	Phase Diagram	103
	7.3	Temperature Dependence of Physical Quantities	106
	7.4	Magnetic Field Switching of Charge Disproportionation	107
	7.5	Discussion and Summary	110
8	Inv	ersion Symmetry Broken State on a Pyrochlore Lattice	111
	8.1	Model and Method	111
		8.1.1 Spin-Ice Double-Exchange Model	112
		8.1.2 Perturbation Theory	113
		8.1.3 Monte Carlo Simulation for the Effective Ising Spin Model	113
		8.1.4 Monte Carlo Simulation for the Double-Exchange Model	114
		8.1.5 Physical Quantities	114
	8.2	Effective Spin Model	116
		8.2.1 J_1 - J_2 - J_3 Ising Model	116
		8.2.2 Monte Carlo Simulation	116
		8.2.3 Emergent Frustration Induced by Further Neighbor In-	
		teractions	118
	8.3	Monte Carlo Study of the Double-Exchange Model	119
	8.4	Spin Hall Effect	121
	8.5	Discussion and Summary	122

A Benchmark of the Polynomial Expansion Monte Carlo						
	\mathbf{Method}	129				
A.1	Model and Parameters	129				
	A.1.1 Spin-Ice Kondo Lattice Model	130				
	A.1.2 Details of the Calculation and Physical Quantities	130				
A.2	Overview of Monte Carlo Calculations	131				
A.3	Convergence in Terms of the Number of Polynomials	133				
A.4	Convergence in Terms of the Truncation Distance	137				
A.5	Convergence in Terms of the Truncation Distance in Larger					
	Systems	139				
A.6	Discussion	140				
A.7	Summary	141				