

# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Geometrical frustration . . . . .	1
1.2	Ice-rule local constraint . . . . .	2
1.3	Purpose of this study . . . . .	5
1.4	Organization of this thesis . . . . .	6
<b>2</b>	<b>Metal insulator transition of charge frustrated systems</b>	<b>7</b>
2.1	Introduction: transport phenomena in itinerant ice-rule systems . . . . .	7
2.1.1	Manganite and Verwey transition . . . . .	7
2.1.2	Metal-insulator transition in molybdenum pyrochlore oxides . . . . .	10
2.1.3	Metal-insulator transition in iridium pyrochlore oxides . . . . .	14
2.2	Model and method . . . . .	16
2.2.1	Model . . . . .	16
2.2.2	Arithmetic mean approximation within the ice-rule manifold . . . . .	16
2.2.3	Lifting of the ground state degeneracy . . . . .	18
2.2.4	Numerical calculations . . . . .	19
2.2.5	Lattices . . . . .	21
2.3	Results . . . . .	21
2.3.1	Pyrochlore lattice . . . . .	21
2.3.2	Checkerboard lattice . . . . .	25
2.3.3	Kagome lattice . . . . .	30
2.4	Discussion . . . . .	33
2.5	Summary of this chapter . . . . .	34
<b>3</b>	<b>Transverse-field Ising model on frustrated checkerboard lattice</b>	<b>37</b>
3.1	Transverse-field Ising models on frustrated lattices . . . . .	37
3.1.1	Triangular lattice . . . . .	37
3.1.2	Checkerboard lattice . . . . .	39
3.2	Model and method . . . . .	40
3.2.1	Transverse-field Ising model on a checkerboard lattice . . . . .	40
3.2.2	Quantum Monte Carlo method . . . . .	41
3.2.3	Continuous-time algorithm . . . . .	43
3.2.4	Loop algorithm and replica-exchange algorithm . . . . .	44
3.2.5	Physical quantities and order parameters . . . . .	44
3.3	Results and discussions . . . . .	45
3.3.1	Effects of external fields in the case of $J_1 = J_2$ and $J_3 = 0$ . . . . .	45
3.3.2	Entropy driven Neel transition . . . . .	48
3.4	Summary of this chapter . . . . .	48
<b>4</b>	<b>Ferroelectric transition of squaric acid crystals</b>	<b>51</b>
4.1	Squaric acid crystal . . . . .	51
4.1.1	Structure and key features: geometrical frustration and quantum fluctuation . . . . .	51
4.1.2	Antiferroelectric transition . . . . .	52
4.1.3	Effect of external pressure . . . . .	53
4.1.4	Effect of deuteration . . . . .	54

4.2	Theoretical models and previous studies . . . . .	55
4.2.1	Pseudospin model . . . . .	55
4.2.2	Vertex model: frustration in squaric acid crystal . . . . .	57
4.3	Model and method . . . . .	59
4.3.1	Model . . . . .	60
4.3.2	Quantum Monte Carlo method . . . . .	61
4.4	Results . . . . .	62
4.4.1	Ferroelectric transition and crossover . . . . .	62
4.4.2	Phase diagram . . . . .	63
4.5	Discussion . . . . .	63
4.6	Summary of this chapter . . . . .	64
<b>5</b>	<b>Conclusion</b>	<b>67</b>
<b>A</b>	<b>Exactly solvable models: the Husimi cacti</b>	<b>69</b>
<b>B</b>	<b>Loss of residual entropy in the liquidlike ground state</b>	<b>70</b>