

# Contents

<b>Acknowledgement</b>	<b>i</b>
<b>Abstract</b>	<b>ii</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Quantum spin liquid . . . . .	1
1.2 Kitaev model . . . . .	4
1.3 Experimental search for Kitaev quantum spin liquids . . . . .	6
1.4 Finite-temperature study of the Kitaev model . . . . .	8
1.5 Purpose of this thesis . . . . .	10
1.6 Organization of this thesis . . . . .	11
<b>2 Model</b>	<b>15</b>
2.1 Hyperoctagon lattice . . . . .	15
2.2 Kitaev model on the hyperoctagon lattice . . . . .	17
<b>3 Method</b>	<b>20</b>
3.1 Majorana fermion representation of the Kitaev model . . . . .	20
3.2 Quantum Monte Carlo method . . . . .	23
3.3 Green-function based kernel polynomial method . . . . .	24
3.3.1 Local update by Green functions . . . . .	24
3.3.2 Kernel polynomial expansion of local Green functions . . . . .	26
3.4 Replica exchange method . . . . .	27
3.5 Boundary conditions . . . . .	27
3.6 Benchmark . . . . .	28
<b>4 Result</b>	<b>35</b>
4.1 Details of numerical simulation . . . . .	35
4.2 Thermal fractionalization . . . . .	36
4.2.1 Specific heat and entropy . . . . .	36
4.2.2 Spin correlations . . . . .	37
4.2.3 Static gauge fluxes . . . . .	38
4.3 “Liquid-gas” phase transition . . . . .	38
4.3.1 Low- $T$ anomaly in the specific heat . . . . .	38

4.3.2	Fluctuation of static gauge fluxes . . . . .	43
4.3.3	Wilson loop . . . . .	43
4.3.4	Critical temperature . . . . .	44
<b>5</b>	<b>Discussion</b>	<b>50</b>
5.1	Ground state . . . . .	50
5.2	Toric-code limit . . . . .	50
5.3	Origin of the “liquid-gas” phase transition . . . . .	51
5.4	Comparison of the critical temperatures between the hyperhoneycomb and hyperoctagon cases . . . . .	52
<b>6</b>	<b>Summary</b>	<b>55</b>