

# Table of contents

<b>Acknowledgement</b>	<b>i</b>
<b>Abstract</b>	<b>iii</b>
<b>List of publication</b>	<b>vii</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Machine learning and physics . . . . .	1
1.2 Neural networks . . . . .	2
1.3 Automatic differentiation . . . . .	3
1.4 Approximating many-body wave functions with neural networks . . . . .	5
1.4.1 Variational Monte Carlo methods . . . . .	5
1.4.2 Neural quantum states . . . . .	7
1.4.3 Neural quantum states of fermionic systems . . . . .	8
1.4.4 Sign problem in fermionic systems . . . . .	10
1.5 Inverse problem in materials science . . . . .	11
1.5.1 Previous studies and their limitations . . . . .	12
1.6 Purpose of this thesis . . . . .	13
1.7 Organization of this thesis . . . . .	14
<b>2 Approximation of fermionic many-body wave functions without using Slater determinant</b>	<b>15</b>
2.1 Method . . . . .	16
2.1.1 Overall framework . . . . .	16
2.1.2 Markov chain Monte Carlo sampling and reweighting . . . . .	18
2.1.3 Generation of states required for energy calculations . . . . .	18
2.1.4 Symmetry operation and representative states . . . . .	19
2.1.5 Neural networks . . . . .	19
2.1.6 Update neural network parameters . . . . .	21

**x | Table of contents**

2.1.7	Computational cost . . . . .	22
2.2	Model and setup . . . . .	23
2.2.1	Hubbard model . . . . .	23
2.2.2	Computational details . . . . .	23
2.3	Results . . . . .	24
2.3.1	Efficiency of reweighting . . . . .	24
2.3.2	Efficiency of two neural networks . . . . .	24
2.3.3	Efficiency of energy variance . . . . .	26
2.3.4	Efficiency of irreducible representation . . . . .	29
2.3.5	Dependence on neural network parameters and Monte Carlo sample numbers . . . . .	30
2.3.6	Inner structure of neural networks . . . . .	30
2.3.7	Benchmark for the system with $6 \times 6$ sites . . . . .	33
2.4	Summary of this chapter . . . . .	34
<b>3</b>	<b>Approximation of fermionic many-body wave functions by combining convolutional neural network and Slater determinant</b>	<b>35</b>
3.1	Method . . . . .	35
3.1.1	Architecture of neural network . . . . .	35
3.1.2	Overall framework . . . . .	36
3.1.3	Accumulation of parameter gradients . . . . .	37
3.2	Model and setup . . . . .	38
3.3	Results . . . . .	38
3.3.1	Comparison with the methods based on the Slater determinant . . . . .	38
3.3.2	Efficiency of combining a neural network representing correlation effects . . . . .	40
3.4	Summary of this chapter . . . . .	41
3.5	Perspective . . . . .	41
<b>4</b>	<b>Inverse design of a Hamiltonian showing large anomalous Hall effect by automatic differentiation</b>	<b>43</b>
4.1	Framework . . . . .	43
4.1.1	Flowchart . . . . .	43
4.1.2	Details of the optimization . . . . .	45
4.2	Rediscovery of the Haldane model . . . . .	45
4.2.1	Model and setup . . . . .	46
4.2.2	Optimization of model parameters . . . . .	49

4.2.3	Initial condition dependence . . . . .	50
4.3	Discovery of a new Hamiltonian on a triangular lattice . . . . .	50
4.3.1	Model and setup . . . . .	50
4.3.2	Optimization of model parameters . . . . .	53
4.3.3	Initial condition dependence . . . . .	56
4.3.4	Refinement of model parameters . . . . .	58
4.4	Summary of this chapter . . . . .	59
<b>5</b>	<b>Inverse design of a Hamiltonian showing large photovoltaic effect by automatic differentiation</b>	<b>61</b>
5.1	Model and setup . . . . .	61
5.1.1	Spin-charge coupled system . . . . .	61
5.1.2	Photocurrent under solar radiation . . . . .	63
5.2	Results . . . . .	65
5.2.1	Optimization process . . . . .	65
5.2.2	Band engineering with automatic optimization . . . . .	66
5.2.3	Initial parameter dependence . . . . .	66
5.2.4	Filling dependence . . . . .	68
5.3	Summary of this chapter . . . . .	70
5.4	Perspective . . . . .	70
<b>6</b>	<b>Conclusion</b>	<b>73</b>
<b>References</b>		<b>77</b>