

ABSTRACT

Title of Dissertation: QUANTUM SIMULATION
OF THE BOSONIC SYSTEM
AND APPLICATION OF MACHINE LEARNING

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First, we introduce the notion of "generalized bosons," whose exchange statistics resemble those of bosons, but the local bosonic commutator $[a_i, a_i^\dagger] = 1$ is replaced by an arbitrary single-mode operator that is diagonal in the generalized Fock basis. Examples of generalized bosons include boson pairs and spins. We consider the analogue of the boson sampling task for these particles and observe that its output probabilities are still given by permanents, so the results regarding the difficulty of sampling carry over directly. Finally, we propose implementations of generalized boson sampling in circuit-QED and ion-trap platforms.

In the rest of the thesis, we move on to different topics. Firstly, we incorporate machine learning techniques in quantum information. We use machine learning to classify rational two-dimensional conformal field theories (CFTs). We first use the energy spectra of these minimal models to train a supervised learning algorithm. In

contrast to conventional methods that are typically qualitative and involve system size scaling, our method quantifies the similarity of the spectrum of a system at a fixed size to candidate CFTs. Such an approach allows us to correctly predict the nature and value of critical points of several strongly correlated spin models using only their energy spectra. Our results are also relevant for the ground-state entanglement Hamiltonian of certain topological phases of matter described by CFTs. Remarkably, we achieve high prediction accuracy by only using the lowest few Rényi entropies as the input. Finally, using autoencoders, an unsupervised learning algorithm, we find a hidden variable that has a direct correlation with the central charge and discuss prospects for using machine learning to investigate other conformal field theories, including higher-dimensional ones.

Next, we demonstrate how machine learning techniques, especially unsupervised learning algorithms, can be used to study Symmetry-Protected Topological (SPT) phases of matter. SPT phases are short-range entangled phases of matter with a non-local order parameter that are preserved under a local symmetry group. Here, we use an unsupervised learning algorithm, namely diffusion maps, to differentiate between symmetry-broken phases and topologically ordered phases and between non-trivial topological phases in different classes. Specifically, we show that phase transitions associated with these phases can be detected in various bosonic and fermionic models in one dimension, including the interacting SSH model, the AKLT model and its variants, and weakly interacting fermionic models. Our approach provides a cost-effective computational method for detecting topological phase transitions associated with SPT systems, which can also be applied to experimental data obtained from quantum simulators.

QUANTUM SIMULATION OF THE BOSONIC SYSTEM AND APPLICATION OF MACHINE LEARNING

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Dedication

Dedicated to my dearest mom and dad, who have been standing behind me.

Acknowledgments

First and foremost, I would like to express my deep gratitude to my supervisor, Mohammad Hafezi, for his continuous support and guidance throughout my Ph.D. studies. I could not have completed this thesis without his help. I know his office door is always open whenever I have any questions about science or life. I would also like to thank Maissam Barkeshli, Victor Albert, Alexey Gorshkov, and Amin Gholampour for their valuable feedback on the early drafts of this thesis.

I am lucky to be surrounded by gifted colleagues as I pursue my graduate studies. We come from all over the world and bring a wealth of different experiences and perspectives to our work. This diversity of thought is essential to generating new ideas and approaches to our research. We are constantly challenging and pushing each other to think outside the box. In addition, we are always there to support and encourage each other when things get tough. I know that I would not be where I am today without the help and guidance of my talented colleagues. Together, we are making groundbreaking discoveries that will have a lasting impact on our field.

I had a fantastic time with my friends during my college days at College Park. I'll never forget it. I want to give special thanks to everyone who made it possible. They have always been there for me, whether I needed someone to talk to or just a shoulder to cry on. They listened to me when I needed to vent and offered sage advice when I was feeling

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Table of Contents

Dedication	ii
Acknowledgements	iii
Table of Contents	v
List of Tables	vii
List of Figures	viii
List of Abbreviations	xi
Chapter 1: Introduction	1
1.1 Motivation	1
1.2 Boson Sampling	2
1.3 Machine Learning Application on Quantum Physics	3
1.4 Conformal Field Theory	4
1.5 Symmetry-Protected Topological Phases	5
1.6 Overview of the thesis	6
Chapter 2: Generalized Boson Sampling	8
2.1 Introduction	8
2.2 Boson sampling for generalized bosons	12
2.3 General implementation scheme	14
2.4 Circuit-QED implementation	16
2.5 Outlook	20
Chapter 3: Decoding conformal field theories: from supervised to unsupervised learning	22
3.1 Introduction	22
3.2 Critical spin-chains	27
3.3 Unsupervised Learning	33
3.4 Discussion	35
Chapter 4: Unsupervised Learning of Symmetry Protected Topological Phase Transitions	36
4.1 Diffusion Map	39

4.2	Model introduction and results	41
4.3	PCA and k-means algorithm	51
Chapter 5:	Conclusion and Outlook	53
Appendix A:		57
A.1	Generalized Bosons	57
A.2	Bosons sampling with generalized bosons	59
A.3	Gaussian Boson Sampling for Generalized Boson	61
A.3.1	Generalized Coherent States	62
A.3.2	P and Q Functions for Generalized Boson	62
A.3.3	Generalized Gaussian states	65
A.3.4	Gaussian Boson Sampling for Generalized Boson	66
A.4	Trapped-ion Implementation	69
A.4.1	Setup	69
A.4.2	Mode-mixing operation	71
A.5	Circuit-QED implementation	72
A.5.1	Mode-mixing Hamiltonian	72
A.5.2	Fock-state preparation	75
Appendix B:		76
B.1	Two-dimensional conformal field theories	76
B.1.1	Virasoro minimal models	78
B.1.2	$\mathbb{Z}_k$ parafermion CFTs	79
B.1.3	$\mathcal{N} = 1$ superconformal minimal models	80
B.2	Details of the neural network architectures and training	81
B.2.1	Supervised learning with energy spectra	81
B.2.2	Supervised learning with Rényi entropies	82
B.2.3	Unsupervised learning	82
B.3	Preprocessing procedure	83
B.4	Comparison of models trained using different classes	84
B.5	Comparison with the conventional method	84
List of Publications		87
Bibliography		89

List of Tables

2.1	Various generalized bosons and their generalized bosonic algebra, defined in terms of either the function $F(n)$ or $f(n)$, see 2.2. For spin- S boson, the spin operators are $S_x = \sum_{j=1}^{2S} \sigma_x$, $S_y = \sum_{j=1}^{2S} \sigma_y$, $\theta(x)$ is the Heaviside step function which is zero for $x < 0$ and 1 for $x \geq 0$. For q-bosons, N is defined such that $[b_q, N] = b_q$, $[b_q^\dagger, N] = -b_q^\dagger$. $[n]_q = \frac{q^n - q^{-n}}{q - q^{-1}}$, $[n]_q! = \prod_{j=1}^n [j]_q$, N_m is the number operator of m -paraboson.	13
3.1	List of all conformal field theories, i.e. classes, we include in our supervised training. We use color dots to indicate the CFT shown in Figs. 3.2 and 3.3.	27
4.1	Summary of 1D Hamiltonians. H labels Haldane phase. Dimerized phase, Dimer phase, ferromagnetic phase, antiferromagnetic phase, XY phase, valence Bound state, $\mathbb{Z}_2$ symmetry breaking (SB) phase, critical phase. . .	41

List of Figures

2.1	Boson sampling with generalized bosons. (a) Circuit-QED implementation for boson pairs $b_i = a_i^2$ as cavity excitations. The mode-mixing operation is implemented as a non-linear photon-pair tunneling. (b) Trapped-ion implementation of super-spins. Generalized boson (superspin) is encoded in internal atomic states. As described in the text the mode-mixing unitary operation is implemented in a Trotterized way by a sequential application of Molmer-Sorensen [1] laser beams to each pair of ions. In both cases, the final step is to perform local population measurement.	10
3.1	Schematic illustration of the machine-learning algorithms to identify different CFTs. The pre-processed energy spectrum or Renyi entropies are stored into a vector that serves as an input to the algorithms. We consider two scenarios: supervised learning, and unsupervised learning. In the former, labels of the CFT class are provided to a neural network classifier, which predicts the CFT theory that describes the given CFT data. In the latter, we use an autoencoder neural network, which learns an efficient representation of the energy spectra. The first half of the network acts as an encoder that maps the input to a single scalar variable ω , and the second half decodes ω and reconstructs the original input. We find that ω is directly correlated to the central charge.	24
3.2	Predictions of our supervised machine learning approaches on the model H_I spectrum data as a function of the transverse field h . (a) The confidence, i.e entropy, S , of the neural network. (b) The Gaussian distance, d_2 , between the energy spectrum of H_{ISING} and the energy spectrum of the first 9 CFTs in Table 3.1. The numbers in the legend refer to the CFT class.	28
3.3	Predictions of our supervised machine learning approaches on a $H_I(h)$ with $h = 1$ (see Fig. 3.2) plus three-body interaction terms that are controlled by a parameter λ . (a) The entropy of probabilities, S , of the neural network. (b) The Gaussian distance, d_2 , between the energy spectrum of H_T and the energy spectrum of the first 9 CFTs in Table 3.1. The numbers in the legend refer to the CFT class.	29

3.4	Probability of the neural network predicting the correct CFT of the entanglement Hamiltonian for the SLM (TLM), depicted with squares (diamonds), as a function of a number of Rényi entropies included in training samples. The overall accuracy of the network is benchmarked using the test data, shown as dark blue circles.	33
3.5	Unsupervised learning: The hidden variable as a function of the central charge for different CFT families (different colors and markers). We observe that within a family, the one-dimensional hidden variable ω is a monotonous function of the central charge.	35
4.1	Schematic illustration of the machine-learning algorithms to identify different phases. (a) Flowchart of the diffusion maps algorithm. From a given Hamiltonian, (1) one obtains the ground state, and projectively samples from the ground state, (2) forms the diffusion matrix and tunes the hyperparameters, (3) obtains the phase diagram by finding the conspicuous transitions in the number of eigenvalues. (b) Different ground states in a cluster can transform to each other via a diffusion process in the dataset basis.	42
4.2	Phase diagrams of model 1 and 2. Colorbar in (a) and vertical axis in (b) represent the number of eigenvalues larger than $1 - \delta$ (See text). (a) Model 1 is an interacting bosonic SPT model with a topological and trivial phase with phase boundaries at $J = \pm J'$. (b) Model 2 is biquadratic spin chain model whose ground state at $\theta = 1/3$ is the AKLT state. The dashed lines illustrate the phase boundaries obtained via DMRG methods.	44
4.3	Phase diagrams of model 3 and model 4. (a) Model 3 is a variant of the AKLT model which hosts one trivial phase (TRI), two symmetry breaking phases ($\mathbb{Z}_2^y$, and $\mathbb{Z}_2^x$), and one topologically ordered phase (Haldane). The topological classification of the system is described by the $\mathbb{Z}_2$ group. The dashed line shows the approximate boundaries of the Haldane phase obtained via exact methods. (b) Model 4 is a weakly interacting fermionic model with unconventional pairing. C labels the states via their distinct zero modes in different phases which is obtained via exact diagonalization. Colorbars represent the number of eigenvalues larger than $1 - \delta$ (See text).	46
4.4	Phase diagram of Hamiltonian in Eq.4.7 in terms of λ, D obtained via the diffusion maps algorithm. Dashed lines represent the exact phase boundaries obtained by DMRG methods.	50
4.5	Phase diagram of Hamiltonian in Eq.4.8 in terms of β, ω obtained via the diffusion maps algorithm. Dashed lines represent the exact phase boundaries obtained by DMRG methods.	51
4.6	PCA and k means on model 3	52
B.1	We use a similar neural network model as in Fig. 2(a) in the main text, but train with different number of classes. The peak at $h = 1$ is stable in different models.	84

B.2 (a) Scaling of the entanglement entropy S in the ground state at a conformal critical point as a function of the system size L . The slope of the linear-log plot gives the central charge c . (b) Visual comparison of the rescaled energies of a simulated model with predicted CFT energies. The correct CFT is class 1 corresponding to the (A_4, A_3) minimal model. 86

List of Abbreviations

AABS	Standard Boson sampling proposed by Aaronson and Arkhipov
AI	Artificial intelligence
ANN	Artificial neural networks
BQP	bounded-error quantum polynomial time
BPP	bounded-error probabilistic polynomial time
CFT	Conformal field theory
DMRG	Density matrix renormalization group
ED	Exact Diagonalization
ES	Entanglement Entropy
GBS	Gaussian Boson sampling
IP	Interactive polynomial time
MC	Monte Carlo
MIP	Multiple interactive provers
NISQ	Noisy intermediate-scale quantum era
PCA	Principal component analysis
QI	Quantum information
RL	Reinforcement learning
SCFT	Superconformal field theory
SPT	Symmetry Protected Topological
VAE	Variational autoencoder

Chapter 1: Introduction

1.1 Motivation

Quantum simulation is an essential tool for understanding the behavior of quantum systems, which are notoriously difficult to study using classical methods. In particular, simulating the behavior of bosonic systems is a challenging problem due to the inherent difficulty of dealing with particles that can occupy the same quantum state. This is known as the bosonic commutation relation, and it leads to a phenomenon called Bose-Einstein condensation, where a large number of bosonic particles can all occupy the same low-energy state. Simulating such a system requires a representation that can handle the large number of particles involved, and the fact that they can all be in the same state makes this representation highly degenerate. Despite these challenges, simulating bosonic systems is important because they are a fundamental component of many physical systems, from superconductors to ultracold atoms, and understanding their behavior is crucial for advancing our understanding of condensed matter physics, quantum information, and quantum computing. On the other hand, quantum simulations are naturally suited for simulating quantum systems, as they can represent and manipulate quantum states directly.

Bosonic systems are quantum systems that consist of particles that obey bosonic

statistics, such as photons, phonons, and other quasiparticles. Bosonic systems are particularly interesting for quantum simulation because they exhibit a wide range of quantum phenomena, including superposition, entanglement, and interference. Furthermore, bosonic systems are ubiquitous in many fields of science and engineering, including condensed matter physics, quantum optics, and quantum information science.

One area of active research in quantum simulation is the demonstration of quantum supremacy [2, 3, 4], which refers to the ability of a quantum computer to perform a task that is intractable for classical computers [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. One approach to achieving quantum supremacy is to simulate the dynamics of a bosonic system on a quantum computer, which has been demonstrated experimentally using a variety of bosonic systems, including photonic circuits and trapped ions.

1.2 Boson Sampling

Boson Sampling is a quantum computing task that involves using bosons to sample from the output of a specific optical circuit. The concept was first introduced in a 2010 paper by Aaronson and Arkhipov [5], and it is believed to be one of the first tasks that a quantum computer can solve more efficiently than a classical computer.

In Boson Sampling and its variants [5, 6, 7, 20, 21], a set of identical bosons (e.g. photons) is injected into an optical circuit consisting of beamsplitters, phase shifters, and detectors. The bosons then undergo interference as they propagate through the circuit, resulting in a probability distribution of outputs that can be measured by the detectors.

The goal of Boson Sampling is to sample from this output distribution, which is

expected to be intractable for classical computers to compute efficiently. This is because the probability distribution is related to the permanent of a matrix [5, 7, 8, 22, 23, 24], which is a notoriously difficult computational problem for classical computers.

While Boson Sampling does not have any immediate practical applications, it represents an important milestone in the development of quantum technologies. It demonstrates the potential of quantum computers to solve problems that are intractable for classical computers and provides a roadmap for the development of more advanced quantum computing applications in the future.

In the first chapter of this thesis, we will discuss the idea of how to generalize the boson sampling into so-called generalized boson sampling by modifying the commutation relation and show its supremacy.

1.3 Machine Learning Application on Quantum Physics

The fields of machine learning, quantum information, and condensed matter theory are closely intertwined. Machine learning algorithms have been applied to a wide range of problems in quantum information, from quantum state tomography to quantum error correction [25, 26]. In turn, quantum information has provided new insights into the foundations of machine learning, with recent research focusing on using quantum algorithms to speed up classical machine learning tasks. On the other hand, condensed matter theory [27, 28, 29] provides a rich source of physical systems that can be used for exploring the limits of quantum computing and quantum information processing [30, 31, 32]. The study of topological materials, for example, has led to the discovery of

new forms of protected qubits that are resistant to environmental noise [33]. Additionally, the study of quantum phase transitions has provided insights into the behavior of quantum many-body systems that are relevant for both machine learning and quantum information processing. As such, the intersection of these fields has the potential to provide significant insights into both the foundations and applications of quantum computing and information processing [34, 35].

In the rest of the thesis, we will describe two machine learning applications on the different condensed matter systems. One is conformal field theory and one is SPT phase. We briefly give an introduction to both phases.

1.4 Conformal Field Theory

Conformal field theory (CFT) is a branch of theoretical physics that studies the behavior of quantum field theories under conformal transformations. Conformal transformations are those that preserve the angles between points, but not necessarily the distances, and they play an important role in many areas of physics, including string theory [36], condensed matter physics [37, 38], and statistical mechanics.

CFTs are characterized by their symmetry under conformal transformations, which leads to a number of powerful techniques for studying their properties. One of the key features of CFTs is the existence of a stress-energy tensor, which describes the behavior of the system under infinitesimal conformal transformations [39, 40]. The stress-energy tensor can be used to compute the correlation functions of local operators in theory, which encode information about the system's dynamics.

CFTs have applications in a wide range of areas of physics, including high-energy physics, condensed matter physics, and quantum information science. In high-energy physics, CFTs play a key role in the study of string theory [39, 40], which is a theoretical framework for unifying quantum mechanics and general relativity. In condensed matter physics, CFTs are used to describe the behavior of critical systems, such as those that undergo a phase transition [41, 42]. In quantum information science, CFTs are used to study the entanglement properties of many-body quantum systems, which are relevant for quantum computing and quantum communication.

The study of CFTs is an active area of research, with many open questions and challenges. Some of the current research directions in CFT include the study of non-equilibrium dynamics, the exploration of the holographic duality between CFTs and gravity, and the application of CFT techniques to new areas of physics, such as topological phases of matter

1.5 Symmetry-Protected Topological Phases

Symmetry-protected topological (SPT) phases are a class of quantum phases of matter that are characterized by both their topological properties and their symmetries. Topological phases of matter are characterized by their global properties, such as the presence of topological edge modes [43] or the existence of nontrivial topological invariants [44, 45, 46, 47, 48, 49, 50], which are insensitive to local perturbations. Symmetry, on the other hand, is a fundamental concept in physics that describes the invariance of physical laws under certain transformations, such as rotations, translations,

or reflections.

SPT phases are interesting because they exhibit a combination of both topological and symmetry-protected properties. In an SPT phase, the topological properties of the system are protected by the presence of a symmetry [51, 52]. This means that if the symmetry is broken, the topological properties of the system can change, leading to a different phase of matter.

SPT phases have applications in many areas of physics, including condensed matter physics [53, 54, 55, 56, 57, 58], quantum information science, and high-energy physics. In condensed matter physics, SPT phases are used to describe the behavior of systems that exhibit topological insulators and superconductors, which have potential applications in electronics and quantum computing. In quantum information science, SPT phases are used to study the robustness of quantum states under noise and decoherence. In high-energy physics, SPT phases are used to study the properties of topological defects and nontrivial quantum field theories.

The study of SPT phases is an active area of research, with many open questions and challenges. Some of the current research directions in SPT include the study of the interplay between topology and entanglement, the classification of SPT phases in higher dimensions, and the exploration of the relationship between SPT phases and quantum field theory.

1.6 Overview of the thesis

The rest of this thesis is organized follows:

1. Chapter 2 is based on

En-Jui Kuo, Yijia Xu, Dominik Hangleiter, Andrey Grankin, Mohammad Hafezi.

”Boson Sampling for Generalized Bosons.” *Physical Review Research* 4 (4), 043096.

2. In Chapter 3 is based on

En-Jui Kuo, Alireza Seif, Rex Lundgren, Seth Whitsitt, Mohammad Hafezi.

”Decoding conformal field theories: from supervised to unsupervised learning.” *Physical Review Research* 4 (4), 043031

3. In Chapter 4 is based on

En-Jui Kuo, Hossein Dehghani. ” Unsupervised learning of interacting topological and symmetry-breaking phase transitions.” *Physical Review B* 105 (23), 235136.

4. In Chapter 5, I will give a summary of the works presented in this thesis and suggest a possible direction for future research.

Chapter 2: Generalized Boson Sampling

2.1 Introduction

Quantum random sampling protocols allow us to demonstrate an advantage of quantum computational devices over classical computers [2, 3, 4]. In a quantum random sampling protocol the task is to sample from the output distribution of certain random quantum computation. Surprisingly, even if those computations are not universal, the sampling task can in many cases be computationally difficult for classical computers [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19].

This is the case even for random linear-optical computations: In *boson sampling* [5] a uniformly random linear mode transformation is applied to a multi-mode bosonic input state and measured in the photon-number basis. Boson sampling protocols come in many different variants, ranging from the original proposal of [5] with Fock-state input states (FBS), to Gaussian boson sampling (GBS) with Gaussian input states [6, 7, 20] and GBS with threshold detectors [21]. The hardness of simulating those schemes can be traced back to the hardness of computing their output probabilities, which are given by certain polynomials in submatrices of the linear-optical unitary [5, 7, 8, 22, 23, 24]. Importantly, the discovery of GBS has enabled recent experimental demonstrations [4, 59] on much larger scales than is possible for FBS [60] due to the experimental difficulty of Fock state

preparation.

In this Letter, we further extend boson sampling protocols to a wider class of quantum systems. Specifically, we introduce *generalized bosons*, which is a wide class of particles that hold bosonic commutation relations between different sites but have non-bosonic local commutation relations. For generalized bosons, the local standard bosonic commutation relations are replaced by an arbitrary diagonal operator in the local Fock basis. A natural question that we address in this Letter is therefore whether quantum advantage can be demonstrated using those generalized bosonic modes analogously to standard bosons.

Specific instances of generalized bosons were first introduced in Refs. [61, 62, 63] and find applications for solving integrable systems [64, 65, 66, 67] and even interacting bosonic systems via perturbation theory [68]. As we discuss in more detail below, modes obeying generalized commutation relation can also be found in AMO systems. While standard bosons are non-interacting, systems with non-trivial diagonal commutation relations can be viewed as interacting. Examples include conventional spin degrees of freedom, and the so-called paraboson [69, 70] that has recently been studied in ion-trap systems [71]. Below, we present and analyze another variant of generalized bosons in a circuit-QED setup taking the form of boson pairs [72, 73, 74, 75, 76].

Within this framework, we show that boson sampling can be simulated efficiently by generalized bosons using Fock state preparations, occupation number measurements and linear mode mixing. Consequently, all the complexity results for the original boson sampling protocol carry over. While linear mode mixing is naturally implemented in non-interacting systems only, we re-interpret a result by [77] to show an approximate, but

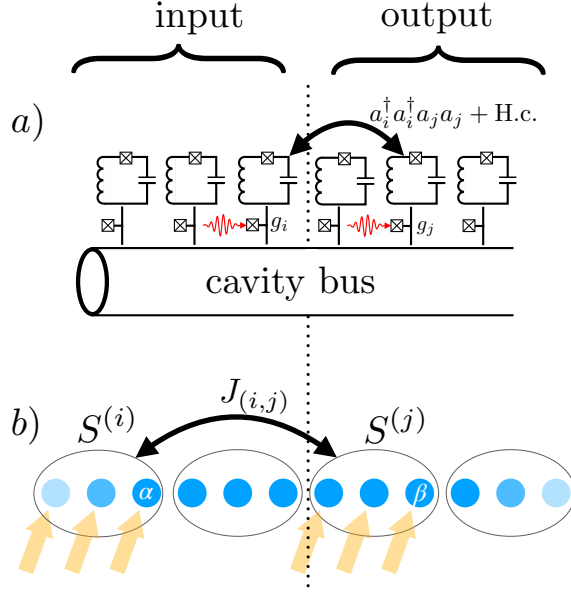


Figure 2.1: Boson sampling with generalized bosons. (a) Circuit-QED implementation for boson pairs $b_i = a_i^2$ as cavity excitations. The mode-mixing operation is implemented as a non-linear photon-pair tunneling. (b) Trapped-ion implementation of super-spins. Generalized boson (superspin) is encoded in internal atomic states. As described in the text the mode-mixing unitary operation is implemented in a Trotterized way by a sequential application of Molmer-Sorensen [1] laser beams to each pair of ions. In both cases, the final step is to perform local population measurement.

efficient, simulation of mode-mixing for generalized bosons, in certain limits. Finally, we provide specific implementation proposals for a circuit-QED and an ion-trap platform.

On a high level, our work can be viewed as addressing the question of whether there is an intermediate system in between qubits and non-interacting standard bosons in terms of the level of interaction. Our results show that performing mode mixing transformations “bypasses” the interactions of generalized bosonic systems, giving rise to the same output probabilities.

Generalized bosons— Let us start by being more specific about the definition of generalized bosonic particles. Recall the standard bosonic commutation relations between

bosonic annihilation and creation operators a_i and $a_i^\dagger$ for a mode i

$$[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i^\dagger, a_j^\dagger] = [a_i, a_j] = 0, \quad (2.1)$$

where $[\cdot, \cdot]$ denotes the commutator and δ_{ij} is the Kronecker delta.

For generalized bosons, the last two commutation relations in 2.2 remain unchanged, while the first commutation relation is modified by multiplying the Kronecker delta by an arbitrary diagonal operator characterized by a function $F : \mathbb{N} \rightarrow \mathbb{C}$ of the single-mode occupation number. Specifically, we define generalized bosonic operators $b_i, b_i^\dagger$ annihilating and creating an excitation in mode i , respectively, by their commutation relations

$$[b_i, b_j^\dagger] = \delta_{i,j} \sum_{n_i=0}^{\infty} F(n_i) |n_i\rangle \langle n_i|, \quad [b_i^\dagger, b_j^\dagger] = [b_i, b_j] = 0. \quad (2.2)$$

Here, the generalized Fock state $|n_i\rangle$ with occupation number n_i in mode i is defined by the action of the creation operator $b_i^\dagger$ on the vacuum as $(b_i^\dagger)^{n_i} |0\rangle = f(n_i) |n_i\rangle$, where $f : \mathbb{N} \rightarrow \mathbb{C}$ is a function that alternatively characterizes the generalized boson. f and F are related and their exact correspondence is discussed in the Supplementary Material [78, Sec. A.1]. For convenience, we call $f(n)$ the *bosonic factor* and only use $f(n)$ in the following. A multimode Fock state of generalized bosons on M modes can thus be written as

$$|n_1, n_2, \dots, n_M\rangle = \left(\prod_{i=1}^M \frac{1}{f(n_i)} \right) b_1^{\dagger n_1} b_2^{\dagger n_2} \dots b_M^{\dagger n_M} |0\rangle. \quad (2.3)$$

We give some examples of generalized bosons and their corresponding bosonic factors in

section 4.1.

The basic idea of the FBS protocol due to [5] is to send a Fock state of N photons in M modes into a uniformly random linear mode-mixing circuit described by a unitary matrix $\Lambda \in U(M)$, and subsequently, to measure the output state in the Fock basis. The linear optical network Λ performs mode-mixing so that the input mode operators $\{a_i\}_{i=1}^M$ are transformed to output operators $\tilde{a}_i = \sum_{j=1}^M \Lambda_{ij} a_j$. The probability of obtaining an outcome $\mathbf{k} = (k_1, \dots, k_M)$ given that the input configuration is given by $\mathbf{l} = (l_1, \dots, l_M)$ for $k_i, l_i \in \mathbb{N}$ such that $\sum_i k_i = \sum_i l_i = N$ is then given by

$$\Pr(\mathbf{k}|\mathbf{l}) = \frac{|\text{Perm}(\Lambda[\mathbf{k}|\mathbf{l}])|^2}{(\prod_i l_i!) (\prod_i k_i!)}. \quad (2.4)$$

Here, the permanent Perm of an $N \times N$ matrix $A = (A_{i,j})_{i,j}$ is defined like the determinant but with only positive signs as

$$\text{Perm}(A) = \sum_{\sigma \in \mathbb{S}_N} \left(\prod_{i=1}^N A_{i,\sigma(i)} \right), \quad (2.5)$$

where $\mathbb{S}_N$ is the symmetric group of N elements. Moreover, $\Lambda[\mathbf{m}|\mathbf{n}]$ is an $(N \times N)$ matrix constructed by repeating the i^{th} column of Λ l_i many times, and the j^{th} row k_j many times.

2.2 Boson sampling for generalized bosons

We are now ready to present the main theoretical result of our work, namely, that the output probabilities of sampling from generalized bosons with Fock-state inputs are proportional to the output probabilities of standard FBS.

Boson type	Definition	$F(n)$	$f(n)$
Standard boson	a	1	$\sqrt{n!}$
Boson pair [72, 73, 74, 75, 76]	$b = a^2$	$2 + 8n$	$\sqrt{(2n)!}$
Spin- S boson [79, 80]	$b = S_x - iS_y$	$(n - 2S) \theta(2S - n)$	$\left(\frac{n!(2S)!}{(2S-n)!} \right)^{\frac{1}{2}}$
q -boson [61, 62, 63]	$bb^\dagger - qb^\dagger b = q^N, q \in \mathbb{C}$	$\frac{[n+1]_q!}{[n]_q!} - \frac{[n]_q!}{[n-1]_q!}$	$\sqrt{[n]_q!}$
m -paraboson [69, 70]	$[b, b^\dagger] = 1 + (2m + 1)e^{i\pi N_m}$	$1 + (2m + 1)e^{i\pi n}$	$\prod_{k=1}^n \left(\frac{2k+2m+3}{2} \right)$

Table 2.1: Various generalized bosons and their generalized bosonic algebra, defined in terms of either the function $F(n)$ or $f(n)$, see 2.2. For spin- S boson, the spin operators are $S_x = \sum_{j=1}^{2S} \sigma_x$, $S_y = \sum_{j=1}^{2S} \sigma_y$, $\theta(x)$ is the Heaviside step function which is zero for $x < 0$ and 1 for $x \geq 0$. For q -bosons, N is defined such that $[b_q, N] = b_q$, $[b_q^\dagger, N] = -b_q^\dagger$. $[n]_q = \frac{q^n - q^{-n}}{q - q^{-1}}$, $[n]_q! = \prod_{j=1}^n [j]_q$, N_m is the number operator of m -paraboson.

Theorem 2.2.1. *Consider a linear transformation $\Lambda \in U(M)$ of M modes of a generalized bosonic algebra on those modes with bosonic factor f . Then the probability of measuring outcome $\mathbf{k}$ given a Fock input state $|\mathbf{l}\rangle$ is given by*

$$\Pr(\mathbf{k}|\mathbf{l}) = \left(\prod_{i=1}^N \frac{f(k_i)}{f(l_i)k_i!} \right)^2 |\text{Perm}(\Lambda[\mathbf{k}|\mathbf{l}])|^2. \quad (2.6)$$

We prove the Theorem in the Supplementary Information [78, Sec. A.2]. Consequently, the complexity of FBS for generalized boson remains the same as the complexity in the standard boson case [5]. As it turns out, it is also possible to construct an analogue of the Gaussian phase-space formalism and a corresponding GBS, which however, is highly unnatural for generalized bosons and hence we defer a detailed discussion to the Supplementary Material [78, Sec. A.3]. An alternative approach to this theorem is to define creation and annihilation operators of generalized boson: $b = g(\hat{n})a, b^\dagger = a^\dagger g(\hat{n}), g(n) = \frac{f(n+1)}{f(n)\sqrt{n+1}}$ and reproduce the derivation of FBS of regular boson, where $g(\hat{n})$ can be regarded as a scaling factor acting on regular bosonic

creation/annihilation operators.

We have pointed out that the output probabilities of FBS are essentially unchanged under varying the diagonal commutation relations between the bosons. But does this connection extend beyond being a mathematical curiosity? While the preparation of Fock states, the implementation of a linear-optical mode transformation and a measurement in the Fock basis are natural operations in the context of quantum optics, whether the same is true for generalized bosons is unclear a priori. Vice versa, our result implies that FBS can be implemented whenever those operations are possible. For those platforms, it can then be used as a quantum advantage benchmark to compare their performance in a hard-to-simulate regime with other platforms.

2.3 General implementation scheme

We now describe the main idea of implementing FBS for generalized bosons by generalizing the implementation for a spin- $\frac{1}{2}$ chain due to [77]. While Fock-state preparations and measurements are natural, and for every fixed particle number there exists a unitary that realizes linear mode mixing, it does not seem possible to implement this unitary efficiently in general. Recall that a mode-mixing transformation $\exp(-itH)$ arises naturally for standard bosons evolved for time t under the quadratic Hamiltonian $H = \sum_{i,j=1}^M h_{i,j} a_i^\dagger a_j$ with coefficient matrix $h \in \mathbb{C}^{M \times M}$. In contrast, the non-trivial commutation relation of generalized bosons create arbitrary higher-order terms in the Baker-Campbell-Hausdorff expansion when evolving an operator b_i under a Hamiltonian that is quadratic in the generalized bosonic operators $b_i, b_i^\dagger$. In other words, quadratic

Hamiltonians of generalized bosons are interacting, and vice versa, non-interacting evolution is generated by highly complex Hamiltonians.

The idea of [77] is to prevent those interactions between individual bosons from happening. To achieve this, they perform a space-time mapping, allowing them to swap input modes with output modes in a single oscillation so that there are no collisions during the time evolution. Specifically, they consider a system of $2M$ modes separated into M input and M output modes, which is evolved for a short, constant time under the Hamiltonian

$$H_{\text{BS}} = \sum_{i,j=1}^M (a_{j,\text{out}}^\dagger R_{ji} a_{i,\text{in}} + \text{h.c.}) \quad (2.7)$$

acting on standard bosonic modes with annihilation operators $\{a_{i,\text{in}}\}_{i=1}^M$ and $\{a_{i,\text{out}}\}_{i=1}^M$ on the two halves of the system, respectively. Here $R \in U(M)$ is a unitary matrix. It turns out that evolving the initial Fock state $|\phi(0)\rangle = |\mathbf{1}^M\rangle_{\text{in}} \otimes |0^M\rangle_{\text{out}}$ under this Hamiltonian for time $\pi/2$ results precisely in a state

$$|\phi(\pi/2)\rangle = (-i)^N \prod_{i=1}^N \sum_{j=1}^M \bar{R}_{j,i} a_{j,\text{out}}^\dagger |0\rangle, \quad (2.8)$$

so that a measurement in the Fock basis on the output modes reproduces the boson sampling protocol.

Let us now consider the analogous generalized bosonic Hamiltonian

$$H_{\text{gBS}} = \sum_{i,j=1}^M b_{j,\text{out}}^\dagger R_{ji} b_{i,\text{in}} + \text{h.c} \quad (2.9)$$

evolved for time $\pi/2$ with initial state $|\phi(0)\rangle$ conceived of as a generalized Fock state. Then the generalized bosonic algebra will introduce an error into the output state, since during the time evolution bosons will ‘meet’ and thus experience the non-trivial diagonal commutation relation.

[77] show that for spin-1/2 systems, in the dilute limit of $M \in \Omega(N^4)$ and for initial states with only 0 or 1 particles in a mode will go to zero as $O(N^2/\sqrt{M})$ in Frobenius norm in the asymptotic limit. Importantly, this translates into a total-variation distance bound between the corresponding output distributions of $O(N^2/\sqrt{M})$. Hence, their result can be read as showing that in this regime, the Hamiltonian (2.9) approximately realizes linear mode mixing under the unitary R .

In the following, we devise two possible implementations of the generalized boson sampling protocol by simulating the Hamiltonian (2.9) in circuit-QED and trapped-ion platforms, respectively. Each protocol includes the preparation of a Fock-state of generalized bosons, a simulation of Hamiltonian time evolution under H_{gBS} , and a measurement in the Fock basis of generalized bosons.

2.4 Circuit-QED implementation

We start by considering photon pairs as the generalized boson where the annihilation operator is simply the square of a standard boson annihilation operator: $b_i \equiv a_i^2$ with $[a_i, a_j^\dagger] = \delta_{i,j}$. It is straightforward to show that $[b_i, b_j^\dagger] = \sum_{n_i=0}^{\infty} (2 + 8n_i) |n_i\rangle \langle n_i| \delta_{ij}$. This expression is clearly diagonal in the Fock basis as required by the definition of generalized bosons; see also section 4.1. Although photon pairs have been

generated in various parts of the electromagnetic spectrum, our scheme requires mode-mixing of photon pairs that is *quartic* in the standard bosonic operators. Fortunately, the generation and manipulation of such photon pairs have been extensively studied in circuit-QED systems [72, 73, 74, 75, 76, 81]. In particular, we consider an array of non-linear resonator interacting with a bus waveguide via a non-linear process (see fig. 2.1(a)) as described by the Hamiltonian

$$H_{\text{eff}} = \sum_i g_i a_i^{\dagger 2} c + \text{H.c.} - \Delta c^{\dagger} c - \chi \sum_i a_i^{\dagger} a_i^{\dagger} a_i a_i \quad (2.10)$$

in the frame rotating at the cavity frequency ω_c . Here, χ, g_i and Δ are the circuit parameters defined in the supplementary material, a_i is the cavity annihilation operator and c is the bus bosonic resonator mode annihilation operator satisfying $[c, c^{\dagger}] = 1$. In particular, we assume that the coupling g can be externally controlled. We note that our implementation allows for the dynamical independent laser control of coupling coefficients $g_i = g_i(t)$. By adiabatically eliminating the bus cavity mode, we find the effective Hamiltonian $H_{\text{pair}} = \sum J_{i,j}(t) b_i^{\dagger} b_j$ with the tunneling being $J_{i,j} = g_i(t)g_j^*(t)/\Delta - \chi\delta_{i,j}$. We note that the on-site interaction χ will be ignored in the following as it can be eliminated by either choosing the coupling constants such that $|g_i|^2/\Delta = \chi$ or by coupling to an additional Josephson junction in analogy to [72]. The Hamiltonian H_{pair} is formally equivalent to H_{gBS} required to perform the mode-mixing operation [77]. In the case in which the coefficients g_i are time-independent, the resulting $J_{i,j}$ is only a rank-1 matrix and therefore does not allow for the implementation of an arbitrary unitary mode transformation. A more general interaction pattern can be obtained by, e.g., using a

multimode cavity. Alternatively, due to the independent dynamical control over coupling terms g_i any Hamiltonian can be implemented in a Trotterized fashion as shown in the Supplementary Material [78, Sec. A.5].

We now discuss the Fock-state $b^\dagger |0\rangle$ preparation step of the protocol. Arbitrary Fock-state preparation has been demonstrated experimentally in circuit QED setups [82]. For that, we first assume the non-interacting limit $g_i \rightarrow 0$. In this case in the non-rotating frame the Hamiltonian 2.10 is local and diagonal in the Fock basis $|n_i\rangle$ with eigenvalues $\varepsilon_n = n\omega_c - n(n-1)\chi$. In order to prepare the desired Fock state we now assume the system is initially prepared in the vacuum state $|0\rangle$. The system is then weakly driven with the driving Hamiltonian $H_{\text{dr}} = \Omega_{\text{dr}}/2 \sum_i (a_i \exp(i\omega_{\text{dr}}t) + a_i^\dagger \exp(-i\omega_{\text{dr}}t))$, where ω_{dr} and Ω_{dr} are the frequency and the amplitude of the driving. In the limit of weak driving $\Omega_{\text{dr}} \ll \chi$, upon tuning the driving frequency to the two-photon resonance $\omega_{\text{dr}} = \varepsilon_2/2$, the system undergoes a two-photon Rabi oscillation $|0_i\rangle \rightarrow b_i^\dagger |0\rangle$ with the period given by a two-photon Rabi frequency $\Omega_2 = \sqrt{2}\Omega_{\text{dr}}^2/(4\chi)$.

The leading error in Fock state preparation is due to populating the state $|1\rangle$ with probability $p_1 \leq \Omega_{\text{dr}}^2/(4|\varepsilon_1 - \omega_{\text{dr}}|^2)$. This probability can be minimized by reducing the Rabi frequency, trading off against decoherence. A further improvement may be achieved by employing the adiabatic protocol [83], which assumes control over the detuning of the drive.

The final step of the protocol is the measurement of the photon number distribution. This can be done by standard means, e.g., by employing the quantum nondemolition measurement protocol as experimentally demonstrated in [84, 85]. The fidelity of the measurement is limited by the cavity decoherence.

Trapped-ion implementation— We now discuss implementation of spin- S generalized bosons using a trapped-ion quantum simulator, as schematically shown in Fig. 2.1(b). To this end, we consider a chain of ions in a linear Paul trap [86]. Each ion is considered to be a two-level system $\{|g\rangle_\alpha, |e\rangle_\alpha\}$ with the corresponding transition frequency denoted as ω_{eg} . We encode the super-spin $S^{(i)}$ as collective excitation of a subset of ions $\{\alpha\}_i$ such that the lowering operator can be defined as: $S_\pm^{(i)} \equiv N^{-1/2} \sum_{\{\alpha\}_i} \sigma_\pm^{(\alpha)}$, where N is the number of ions encoding the superspin and $\sigma_-^{(\alpha)} \equiv |g\rangle_\alpha \langle e|$, $\sigma_+^{(\alpha)} \equiv |e\rangle_\alpha \langle g|$.

We split our implementation into three steps: state preparation, unitary mode mixing via 2.8, and measurement. The initial superspin Fock (Dicke)-state preparation can be performed using the technique experimentally demonstrated in Ref. [87]. It consists of two steps: first the preparation of the motional Fock state by selectively driving the first motional blue sideband. The second step consists of driving the target superspin ions resonantly with the red motional sideband thereby transferring the excitation into the Dicke state $N^{-1/2} \sum_{\{\alpha\}_i} |e\rangle_\alpha$.

We now discuss a Trotterized way [88] of implementing time evolution under the long-range Heisenberg-exchange type interaction $H_{\text{int}} = J_{(i,j)} S_+^{(i)} S_-^{(j)} + \text{H.c.}$ featuring in the Hamiltonian (2.7). As extensively discussed in the literature [89], such an interaction between any pair of ions can be generated driving ions in a generalized Mølmer-Sorensen [1], with tailored laser configuration [90]. More precisely, we consider a pair of bichromatic laser beams driving the transition $e \leftrightarrow g$ with the laser frequencies respectively tuned to $\omega_{eg} + \Delta$ and $\omega_{eg} - \Delta$ where Δ is laser detuning. As we discuss in the Supplementary Material [78, Sec. A.4] this generates the ion-ion interaction characterized by the Hamiltonian $H_{(\alpha,\beta)}^{(XY)} \approx J^{(\alpha,\beta)} \{\sigma_+^{(\alpha)} \sigma_-^{(\beta)} + \text{H.c.}\}$, where the interaction coefficient

scales as $J_{(\alpha,\beta)} = J_0/|\alpha - \beta|^\zeta$ with $0 < \zeta < 3$ and J_0 is interaction constant. We note that a complex-valued flip-flop interaction can be achieved by adjusting laser phases. Time evolution under the desired Hamiltonian H_{int} can then be obtained in a Trotterized way by running the interaction $H_{\alpha,\beta}^{(XY)}$ for each pair of ions for a time $\delta t_{\alpha,\beta}$ inverse proportional to the interaction strength $J_{(\alpha,\beta)}$ to preserve the spin symmetry $\delta t_{i,j}^{\alpha,\beta} \approx \delta t_{i,j} \times \tilde{J}/J_{\alpha,\beta}$, where $\tilde{J} = \min_{\{i\}_\alpha \{j\}_\beta} [J_{i,j}]$. To the lowest order in Floquet-Magnus expansion we find:

$$H_{\text{eff}} \approx J_0 N \frac{\sum_{i,j} \delta t_{i,j} \left\{ S_+^{(i)} S_-^{(j)} + \text{H.c.} \right\}}{\sum_{i,j} \sum_{\alpha,\beta} \delta t_{i,j} \times |\alpha - \beta|^\zeta}. \quad (2.11)$$

By performing the summation and assuming the densest unitary operation ($\delta t_{i,j} = \delta t$) for $\zeta \approx 0$ and $N = 2$, corresponding to $S = 1$, we find the interaction between N_S superspins to be of the order $\max(J^{(\alpha,\beta)}) = 4 \times J_0 / (N_S^2 - N_S)$. We note that this scaling can potentially be improved by performing optimization of the Mølmer-Sorensen laser configuration [91]. The number of available superspins can be estimated as $\max(J^{(\alpha,\beta)}) > \gamma$, where the decoherence rate is $\gamma \approx 1\text{Hz}$. By taking $J_0 \approx 1\text{kHz}$ we find the number of available superspins to be of the order of $N_S \approx 50$.

Measurement results in the collective basis can be inferred from just local spin measurements due to the restriction to the collective states of each superspin.

2.5 Outlook

Universal circuit sampling and boson sampling formalize natural notions of random computations in the circuit model and the linear-optical model of computation,

respectively. Viewed from the perspective of generalized bosons, these systems are captured by spins and standard bosons, respectively. In contrast to standard bosons spins are strongly interacting. Our results can be viewed as addressing the question of whether there is an intermediate system between qubits and non-interacting standard bosons in terms of the level of interaction. Indeed, generalized bosons provide a natural framework for thinking about this question and we make some first progress by showing that boson sampling can be simulated in such intermediate systems. Having said that, it is less clear that this is indeed the most natural notion of random computation in these contexts. An exciting open question is thus to identify as well as assess the computational complexity of natural random computations for various physical platforms.

A key open question for generalized boson sampling is the question of whether it is possible to certify samples produced in such models. For standard bosons, state preparations can indeed be verified by making use of the formalism of Gaussian quantum information [92]. As we discuss in more detail in the Supplementary Material [78], this formalism does not carry over to generalized bosons, and it is therefore an interesting open to show how generalized bosonic state preparations can be efficiently verified.

Chapter 3: Decoding conformal field theories: from supervised to unsupervised learning

3.1 Introduction

Conformal field theories (CFT), which are quantum field theories with conformal invariance, appear in many areas of physics including condensed matter, statistical physics, and string theory [39, 40]. This procedure turns out to be especially powerful in two spacetime dimensions (one spatial dimensional and one temporal dimension), where the conformal group is infinite-dimensional, and certain two-dimensional CFTs may be classified by a finite number of primary fields [39, 40]. These CFTs, which are realized in a number of physically relevant systems, including the low-energy theory of the quantum critical point of the transverse-field Ising model [93], the edge states (along with the ground-state entanglement Hamiltonian) of fractional quantum Hall systems [37, 38], and the Polyakov action describing the world sheet in string theory [36], are important for being rare examples of analytically tractable strongly-interacting quantum field theories.

Therefore, given some data of a quantum system, it is important to identify whether that system is described by a CFT. This data, obtained from either experimental measurements or numerical simulations, could be the few lowest energy levels of a

given Hamiltonian or Rényi entanglement entropies, which can be measured by probing multiple copies of the system’s state [94, 95, 96, 97, 98]. In particular, it is interesting to ask if this information can be used to detect whether a system is at a critical point, and what kind of CFT describes it the best. To address this question, we turn to machine learning.

Machine learning has been increasingly used to study a wide range of problems in different areas of physics over the past few years [99]. Notable examples include: classifying phases of matter [27, 28, 29], studying non-equilibrium dynamics of physical systems [30, 31, 32], studying the string theory landscape [100] and AdS/CFT correspondence [101], simulating dynamics of quantum systems[33], quantum state tomography [25, 26], and augmenting capabilities of quantum devices [34, 35].

In this work, we use both unsupervised and supervised machine learning to investigate various two-dimensional CFTs, as sketched in Fig.3.1. For supervised learning, we use a deep neural network. Our first training data set is the lowest energy levels of exactly-solvable two-dimensional CFTs. The chosen CFT models include the well-known Ising critical point and $SU(2)_k$ anyonic chain parafermionic model (see Table 3.1 for a full list). We then ask the machine to locate and predict the nature of critical points of quantum spin-chains to high accuracy. By looking at the confidence of the network, we are able to correctly identify the value of the critical point. Remarkably, our approach requires a single system size, whereas common methods (such as entanglement scaling [102]) require finite-size scaling. We further elaborate on the advantage of our method compared to conventional methods and provide examples in the Supplementary Material. Given that the entanglement spectra (ES) of various topological phases of

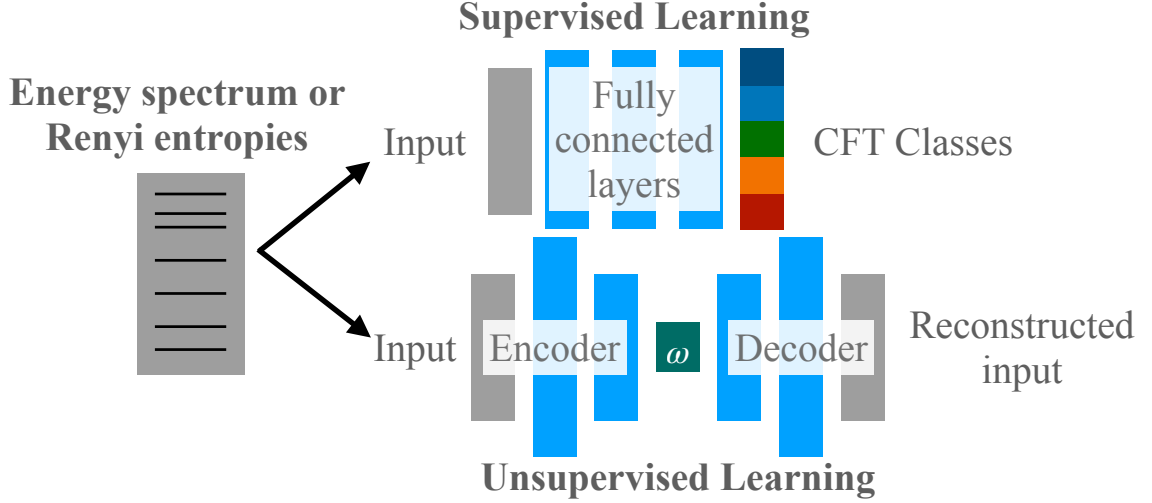


Figure 3.1: Schematic illustration of the machine-learning algorithms to identify different CFTs. The pre-processed energy spectrum or Rényi entropies are stored into a vector that serves as an input to the algorithms. We consider two scenarios: supervised learning, and unsupervised learning. In the former, labels of the CFT class are provided to a neural network classifier, which predicts the CFT theory that describes the given CFT data. In the latter, we use an autoencoder neural network, which learns an efficient representation of the energy spectra. The first half of the network acts as an encoder that maps the input to a single scalar variable ω , and the second half decodes ω and reconstructs the original input. We find that ω is directly correlated to the central charge.

matter are also described by CFTs [38, 103], we train our network with the lowest few Rényi entropies. While the relationship between Rényi entropies and ES is non-linear and requires all Rényi entropies to solve for the ES exactly, we are able to extract the CFT that describes the ES of two different spin-ladder systems to high accuracy with only having access to the lowest few Rényi entropies. Finally, we use the autoencoder algorithm [104], i.e. an unsupervised learning algorithm, and we find that the value of the hidden variable is directly related to the central charge. This gives us a hint that the machine can detect the complexity of CFTs.

Machine learning and CFT basics.—We first review the CFT knowledge needed to generate our training data (see Ref. [39] for a detailed review of CFTs and Ref. [104] for

machine learning), which is taken to be the lowest twenty energy levels of a finite-size model. We take our system to have periodic boundary conditions, although our approach can be readily generalized to include other boundary conditions. In this work, we restrict ourselves to rational CFTs (RCFTs), which only contain a finite number of primary fields, and we furthermore focus on CFTs with field content such that they are modular invariant (see the Supplementary Material [B.1](#) for definitions and details). Our methods may easily be applied to CFTs with non-modular invariant field content.

The discrete energy levels (in units of $2\pi/L$, where L is the length of the system, and $\hbar = 1$) of a generic finite one-dimensional model which flows to a CFT is given by [\[39\]](#)

$$E = E_1 L + E_0 + \frac{2\pi v}{L} \left(-\frac{c}{12} + h_L + h_R \right), \quad (3.1)$$

where E_1 , E_0 , and v are non-universal constants, and c is the central charge of the CFT. We are also omitting subleading dependence on L due to corrections to the scaling limit. Here, $h_L = h_L^{(0)} + m_L$ and $h_R = h_R^{(0)} + m_R$, where $h_L^{(0)}, h_R^{(0)}$ correspond to scaling dimension of the primary fields and m_L and m_R are non-negative integers describing the descendant fields.

As a definite example, we now discuss the structure of the primary descendant fields for the critical Ising model, the simplest non-trivial CFT, and an example of a Virasoro minimal model. With modular invariance imposed, there are three primary fields for this model, $h_{L,R}^{(0)} = 0, \frac{1}{16}$ and $\frac{1}{2}$. The number of descendant fields can be calculated by expanding the so-called character function, as reviewed in the Supplementary Material . Upon doing so, one finds the lowest ten energy levels of this CFT (with the ground state

energy set to zero) are $\frac{2\pi v}{L} \times \{0, \frac{1}{8}, 1, \frac{9}{8}, \frac{9}{8}, 2, 2, 2, 2, \frac{17}{8}\}$. The energy spectrum of some of the other models we consider are discussed in the Supplemental Material, and the list of all CFTs we consider for unsupervised learning is given in Table 3.1. We stress that this is by no means a complete list of RCFTs, as there are actually an infinite number of them.

We use a neural network to classify the input CFT spectra into their corresponding CFT classes (see Fig. 3.1). Specifically, we use a multilayer perceptron (MLP) with with the input and output being the first 15 energy levels and their corresponding CFT class labels from the 13 CFT classes in Table 3.1 (see Supplementary Material for a discussion on the stability of the network with respect to different number of classes). For the training, we optimize the categorical cross entropy over samples of the pre-processed energy spectra of different CFT classes with their corresponding labels. The pre-processing step, which transforms the input such that the ground state energy is set to zero and the other energies are rescaled so that largest energy level is 1 is crucial as it removes the contributions of the non-universal constants in the input data (see Supplementary Material).

Note that conventional methods for identifying CFTs require data from different system sizes to extract the central charge and universal part of the spectrum. In particular, the central charge can be obtained from the scaling of the entanglement entropy in the ground state with the system size. The CFT class can then be identified by visually comparing the energy spectrum of the system with the predicted spectra of different CFT classes consistent with the obtained central charge [105, 106]. In contrast, our method only requires the spectrum at fixed system size, encompasses all the above steps in single black box, and returns the CFT class corresponding to the input data. Note that using

Model	Class	Central charge
(A_3, A_2) - Ising	0 ●	$1/2$
(A_4, A_3) - Tricritical	1 ●	$7/10$
(D_4, A_4)	2 ●	$4/5$
(A_6, D_4)	3 ●	$6/7$
$\mathbb{Z}_4$ parafermion	4 ●	1
$\mathbb{Z}_5$ parafermion	5 ●	$8/7$
$\mathbb{Z}_6$ parafermion	6 ●	$5/4$
$N = 1$ SCFT, $k = 5$	7 ●	$81/70$
$N = 1$ SCFT, $k = 7$	8 ●	$55/42$
$(A_{k+1}, A_k), k = 5 - 8$	9 - 12	$1 - 6/(k(k+1))$

Table 3.1: List of all conformal field theories, i.e. classes, we include in our supervised training. We use color dots to indicate the CFT shown in Figs. 3.2 and 3.3.

this method, the CFT type is not uniquely identified by looking at the spectrum at a fixed system size. The output of the algorithm is the most likely CFT in its library that describes the input spectrum. (see also Supplementary Material for a more detailed comparison).

3.2 Critical spin-chains

We now use the network trained on ideal CFT energy spectra with added noise, to make predictions for two physical models. Specifically, we feed the machine energy spectra from two many-body quantum spin models obtained using exact diagonalization. By analyzing the output of the machine, we are able to predict the location of the critical point and the type of CFT that describes it.

We first consider the transverse Ising model, $H_I(h) = -\sum_{i=1}^L \sigma_i^z \sigma_{i+1}^z - h \sum_{i=1}^L \sigma_i^x$. Here, σ_α^i are the Pauli matrices on-site i and h is a global magnetic field. For $h = 1$, the low-energy theory of H_I is a CFT whose central charge is $c = 1/2$ (minimal model

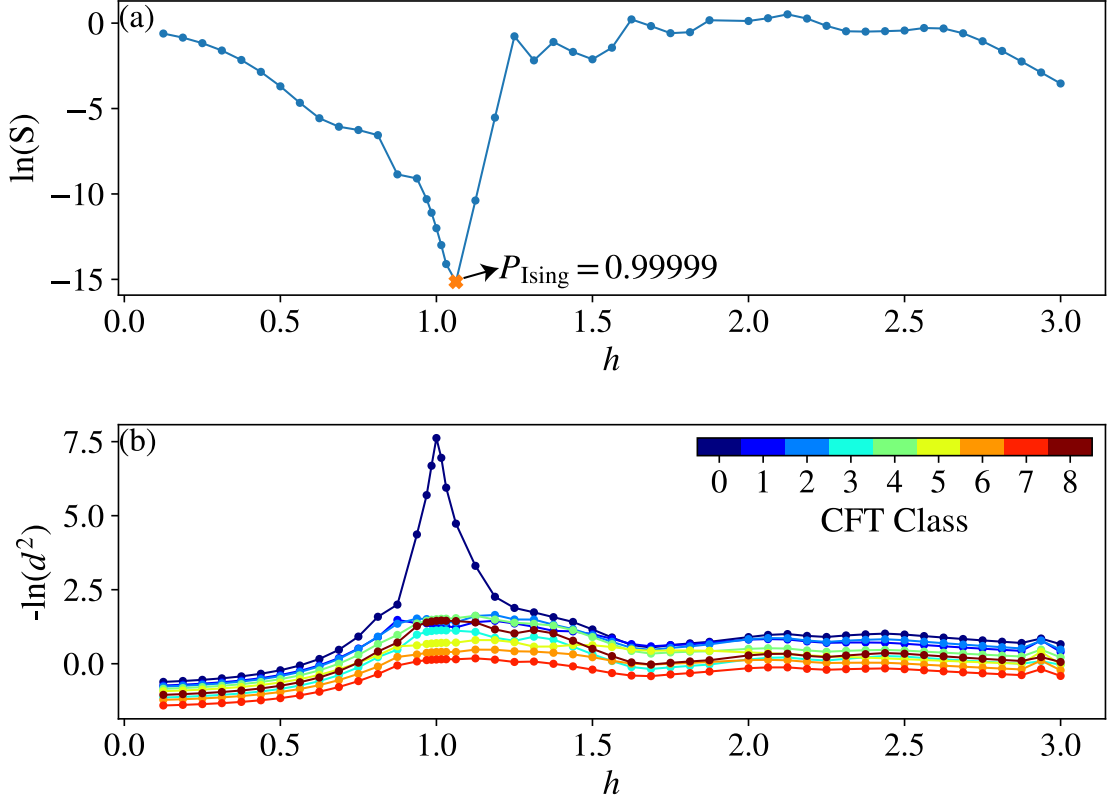


Figure 3.2: Predictions of our supervised machine learning approaches on the model H_I spectrum data as a function of the transverse field h . (a) The confidence, i.e entropy, S , of the neural network. (b) The Gaussian distance, d_2 , between the energy spectrum of H_{ISING} and the energy spectrum of the first 9 CFTs in Table 3.1. The numbers in the legend refer to the CFT class.

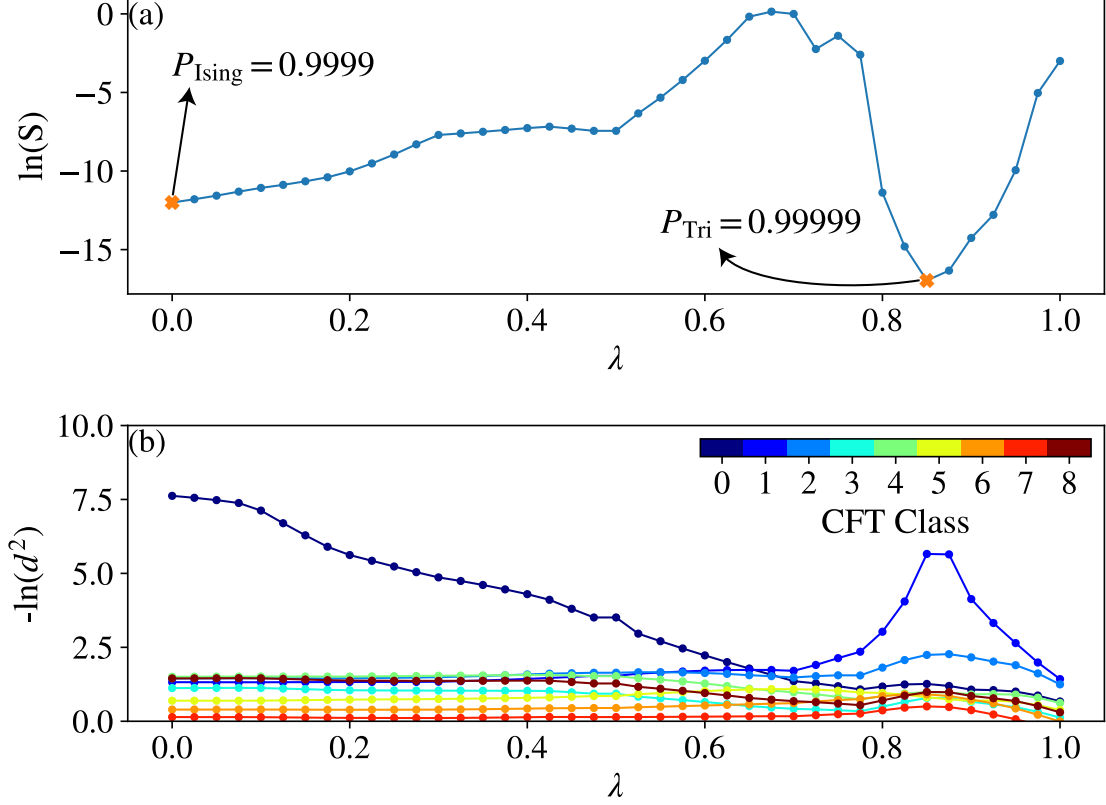


Figure 3.3: Predictions of our supervised machine learning approaches on a $H_I(h)$ with $h = 1$ (see Fig. 3.2) plus three-body interaction terms that are controlled by a parameter λ . (a) The entropy of probabilities, S , of the neural network. (b) The Gaussian distance, d_2 , between the energy spectrum of H_T and the energy spectrum of the first 9 CFTs in Table 3.1. The numbers in the legend refer to the CFT class.

(A_3, A_2)). We perform exact diagonalization (for $L = 22$) for different h and feed the energy spectrum into the network. In Fig. 3.2a, we observe that the entropy S of the output layer, $S = -\sum_i p_i \ln p_i$, where p_i corresponds to the i -th value of the output softmax layer, is minimal at $h = 1$ and has a large probability of being described by minimal model (A_3, A_2) . This indicates that the network has not only correctly predicted the location of the critical point for this model, but also the nature of the critical point, i.e., the CFT class, the central charge, and the primary fields describing the critical point.

Before moving on to the next model, we discuss another quantitative approach to identifying CFTs from energy spectra. We consider a clustering algorithm, using the Gaussian kernel of the Euclidean distance, i.e., $d_2(x, c_m) = e^{-\|x - c_m\|_2^2}$, where x is the input spectra and c_m is the center of the m 'th cluster [104]. In our work, the ideal center of clusters is known from the CFT theory. Therefore, given an energy spectra, we calculate and compare the kernel on the rescaled input and the cluster centers of each CFT. In Fig. 3.2b, we plot d_2 for the Ising model and various CFTs. We observe that d_2 is peaked around the critical point for only the Ising model (Fig 3.2b), similar to the neural network approach (Fig 3.2a). However, we believe the neural network approach will be more reliable as it does not rely on a single energy spectrum.

We now move to a more complicated model, which has two critical points described by different CFTs and both two-body and three-body interactions. The Hamiltonian of this model, originally introduced in Ref. [107], is given by $H_T = 2H_I(1) + \lambda H_3$, where $H_3 = \sum_j \sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^z + \sigma_j^z \sigma_{j+1}^z \sigma_{j+2}^x$. For $\lambda = 0$, this model is described by minimal model (A_3, A_2) as discussed above. When $\lambda \approx 0.856$, the low-energy theory of this model is described by a different minimal model, (A_4, A_3) . Again, we feed the network

the many-body energy spectrum for various λ . In Fig. 3.3a we observe that the machine is correctly able to identify the location and underlying CFTs of the two critical points with high accuracy. Similar results are seen for the Gaussian kernel method (Fig. 3.3b).

Rényi Entropies.— We now consider training with Rényi entropies. This is motivated by the fact that the (bipartite real-space) entanglement Hamiltonian, H_e , of two-dimensional topological phases is often described by (either chiral or non-chiral) one-dimensional CFTs [38, 103]. Unfortunately, it is hard to experimentally measure the eigenvalues of H_e , i.e. the ES (although there are various theoretical proposals on how to do so [108]). Instead, one typically measures the Rényi entropy by preparing multiple copies of the state and interfering with them [96]. Furthermore, one can calculate S_n with quantum Monte Carlo, making the calculation of entanglement more manageable for larger systems [98, 109]. We will demonstrate that, given a critical H_e ¹, one can train neural-networks with Rényi entropies to correctly identify the underlying CFT.

The n -th Rényi entropy is defined as $S_n = \frac{1}{1-n} \ln \text{Tr } \rho_A^n$, where ρ_A is the reduced density matrix and n is some positive integer not equal to one. The ES (eigenvalues of $-\ln(\rho_A)$) can be obtained with knowledge of S_n for all n . In practice one can obtain an estimate of ES with only a finite number of S_n [94, 109]. In these approaches, the ES is obtained from the roots of a polynomial equation, whose coefficients are related to Rényi entropy entropies through Newton’s identities. However, root-finding algorithms are sensitive to errors in the coefficients, making such schemes unstable in the presence of errors in S_n measurements [110]. We approach this problem using machine learning.

¹When H_e is far from criticality, our neural-network occasionally incorrectly predicts the sample data to be in one CFT class with very large probability. This is in sharp contrast to training with energy spectra. It would be interesting to see if this a fundamental problem with Rényi entropies or can be fixed by using more sophisticated techniques such as adversarial training.

If H_e is a CFT, the i th ES level is given by $\epsilon_i = \epsilon_0 + \epsilon_1 L + \frac{2\pi v}{L} n_i$, where n_i is the universal part of the spectrum (see Eq. (3.1)). We remind the reader n_i is a different set of numbers for each respective CFT. S_n , which is only a function of $\frac{v}{L}$ (for a given CFT), can then be written as

$$S_n = (1 - n)^{-1} \ln \left[\left(\sum_{i=0} e^{-n \frac{2\pi v}{L} n_i} \right) / \left(\sum_{i=0} e^{-\frac{2\pi v}{L} n_i} \right)^n \right]. \quad (3.2)$$

We restrict the sum in Eq. (3.2) to the lowest 100 ES levels. For training, we consider a finite range of $\frac{v}{L} \in (0.2, 10)$. This range is chosen not to include large (small) $\frac{v}{L}$ where excited state information is washed out (choice of cut-off plays an important role). Also, note that for larger n , S_n becomes less dependent on the cut-off by definition. Thus, in the chosen range of $\frac{v}{L}$, the choice of cut-off, i.e. simply truncating the sum, has little effect on our results.

Instead of each sample being a vector of energy levels as in the previous section, it is a vector of Rényi entropies, $(S_2, S_3, \dots)$. Here, we include up to 28 Rényi entropies, starting with S_2 . We train our machine with 10000 in different samples for each CFT class (same classes used for energy spectrum training). We generate the data uniformly by randomly choosing $\frac{v}{L}$. We obtain a training accuracy of up to 94 % depending on the number of S_α included. Generally, upon increasing the number of S_α included, the accuracy increases (see Fig. 3.4). See Supplementary Material for details of the networks and training.

We test our model on two exactly-solvable systems studied in Ref. [103]. These are quantum spin ladders which we refer to as the square ladder model (SLM) and triangle

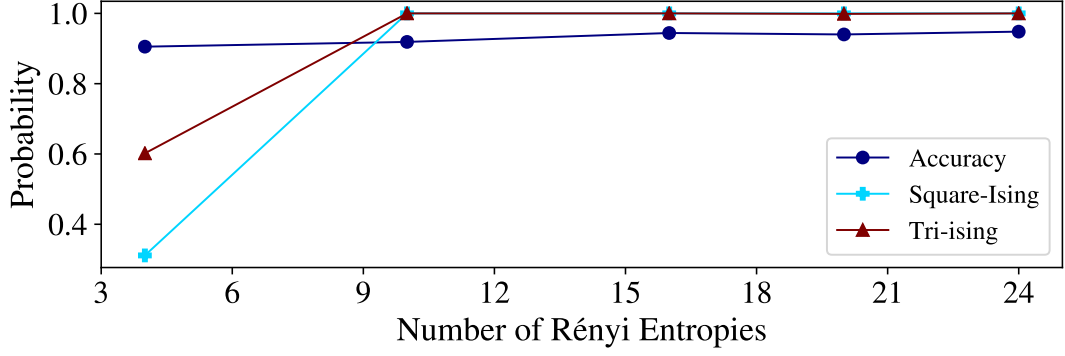


Figure 3.4: Probability of the neural network predicting the correct CFT of the entanglement Hamiltonian for the SLM (TLM), depicted with squares (diamonds), as a function of a number of Rényi entropies included in training samples. The overall accuracy of the network is benchmarked using the test data, shown as dark blue circles.

ladder model (TLM). The ground states of these two models may be written down exactly [103], from which we obtain the reduced density matrix at the critical point. The critical theory of the SLM (TLM) is described by the minimal model (A_3, A_2) $((D_4, A_4))$. We numerically calculate S_n for $L = 18$ and use these numerical results as input into our trained neural-network. We find that the neural-network correctly predicts the CFT that describes H_e for both models with high accuracy. As expected, this accuracy generally increases as one increases the number of S_α included in the training set (see Fig. 3.4).

3.3 Unsupervised Learning

We now turn to using unsupervised learning to explore two-dimensional CFTs. Our data consists of three families of CFTs (see Fig. 3.5 for the list of CFTs used for unsupervised training). We use autoencoders [111] to find a compressed representation of the CFTs (see Fig. 3.1). Previously, autoencoders have been able to detect the order

parameter, i.e. magnetization, in the Ising model [28]. The autoencoder is comprised of an encoder function $\omega = f(\mathbf{x})$ and a decoder function $\mathbf{r} = g(\omega)$, where the hidden variable ω encodes a compressed representation of the input $\mathbf{x}$. The hidden variable is used by the decoder to find the reconstruction $\mathbf{r}$. By restricting the dimension of ω , the network only approximately reconstructs the input, however, it learns the important features of the training data and encodes it in ω . Each class has 100 examples which consists of the lowest 100 energies of the CFT (with same noise added as our energy based classification section.)

We train different autoencoders on a set of energies corresponding to different CFT classes by minimizing $C = \frac{1}{N_m} \sum_m \|\mathbf{r}_m - \mathbf{x}_m\|_2^2$, where the sum is taken over N_m examples in the training set. The x_m is a input of the first layer and r_m is a output of the last layer (see Supplementary Material).

We consider the simplest case of $h = 1$ and show the value of ω for different CFT spectra in Fig. 3.5. We observe that within a single family of CFTs, the magnitude of the hidden variable has positive correlation with k , and hence the central charge.

Finally, we note recent work used supervised machine learning to investigate CFT correlation functions and the emergence of conformal invariance [112]. Recently, it is been demonstrated that for the specific conformal field theory like Ising CFT, one can use an unsupervised learning method to classify them without dimensional reduction [113, 114]. However, the information of the critical point should be known in advance which is different from our work. Our work specifies conformal field theory by using the hidden variable when restricting to a single-family without knowing the critical point in advance. In the future, it would be interesting to include correlation functions in our unsupervised

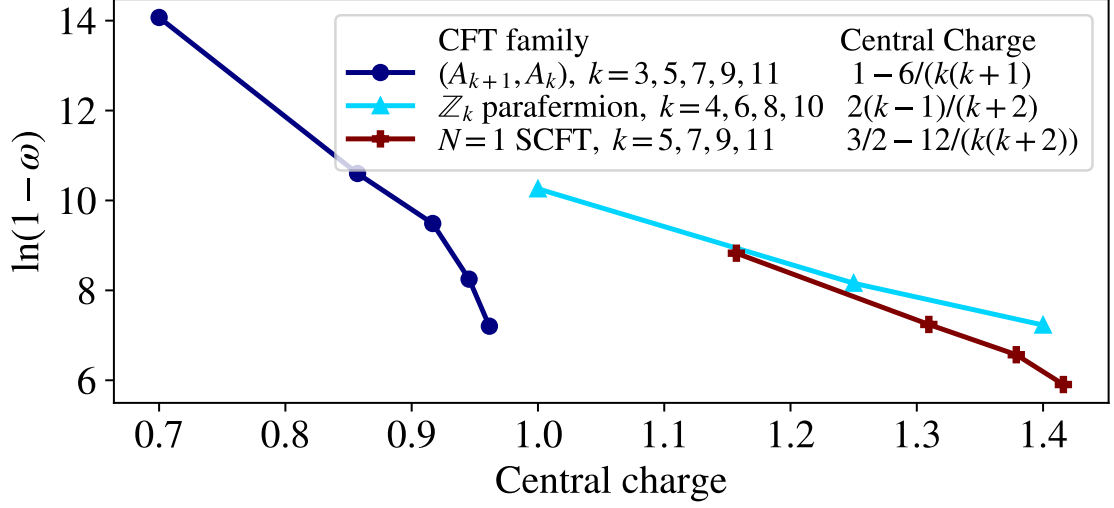


Figure 3.5: Unsupervised learning: The hidden variable as a function of the central charge for different CFT families (different colors and markers). We observe that within a family, the one-dimensional hidden variable ω is a monotonous function of the central charge.

training to see if could distinguish different families of CFTs.

3.4 Discussion

There are several directions where our work can be readily extended. For example, the entanglement Hamiltonian of a CFT can always be written in terms of the boost operator [115, 116], to which our methods may be applied. For critical one-dimensional systems, the entanglement spectra for particular entanglement cuts correspond with the spectra of boundary CFTs [117, 118, 119], which are also known [120, 121, 122]. We believe the methods developed in this Letter can be straight forwardly extended to these CFTs.

Chapter 4: Unsupervised Learning of Symmetry Protected Topological Phase Transitions

Introduction.— In the last two decades, theoretical prediction and experimental observation of topological phases of matter [123] have been one of the most remarkable advancements in the field of condensed matter physics. In topological quantum phases of matter, although, the energy spectrum is gapped, a Landau-Ginzburg framework based on existence of local order parameters, cannot explain some of the most important features of these system such as the existence of symmetry protected edge states [43]. While initially most efforts were mostly focused on non-interacting topological insulators, [44, 45, 46, 47, 48, 49, 50] in recent years, attention has turned into interacting topological phases of matter.

Classifying topological insulators and superconductors which are described by non-interacting fermionic Hamiltonians is less challenging than characterizing interacting topological phases of matter. In particular since the spectrum of non-interacting models are often exactly solvable, classifying them can be done rigorously via several methods including the classification of random matrices [124], Dirac operators [125] or more abstractly via K-theory [126]. Nevertheless, for interacting topological systems, more refined methods such as group cohomology methods have been proposed [51, 52].

Correspondingly, for the former systems, using the wave functions of the Hamiltonian or the Green's functions in the momentum space one can define their corresponding topological invariants, while for the latter, one needs to define non-local order parameters in the real space [53, 54, 55, 56] which is both computationally and experimentally costly to probe [57, 58]. Therefore, identification of topological properties in a given interacting topological systems, is computationally more involved and designing efficient computational methods to detect possible topological phase transitions is an indispensable task for studying these phases.

On the other hand over the past few years machine learning (ML) has emerged as a powerful tool to assist physicists to study a plethora of different problems in condensed matter and quantum sciences. A non-exhaustive list of notable examples include classifying phases of matter [27, 28, 29, 127], studying non-equilibrium dynamics of physical systems [30, 31, 32], simulating dynamics of quantum systems [25, 26, 33], and augmenting capabilities of quantum devices [34, 35]. In particular in classifying applications, most of such techniques rely on supervised ML techniques where the ML algorithms after being trained with labeled systems learns to classify systems with new parameters [27, 32, 128, 129, 130, 131, 132, 133]. However, more interestingly in unsupervised machine no prior knowledge of the phase of the systems is provided and the algorithm by detecting the hidden structure of the input data learns to cluster wave functions or Hamiltonians in different phases [28, 134, 135].

Goal.— In this work, we use unsupervised learning model (ULM), namely the diffusion maps algorithm (DMA), to detect different topological phase transition associated with symmetry protected interacting topological phases with short-range

entanglement also known as symmetry-protected topological (SPT) systems [51]. However, we note that our method can only detect the presence of topological phase transitions and cannot distinguish between different topological phases. The diffusion map algorithm which can capture the hidden geometrical and topological structure of data sets [136, 137], recently, has been used to classify phases of matter in the local order of the Ising model [138], thermal topological vortex structures and temperature driven phase transitions [139, 140], and non-interacting topological insulators [141, 142, 143].

Here, by applying this algorithm to different bosonic and fermionic systems in one dimension which host SPT phase, we demonstrate that this technique can approximately identify topological phase transitions and reproduce the phase diagram of models which in addition to symmetry broken phases can host one or several interacting SPT phases. Hence, in systems where based on physical symmetry arguments, it is known that there are finite possibilities for the formation of symmetry broken phases, detection of additional phases via our method is an evidence that the system can host non-trivial SPT phases. We should highlight that since we only need snapshots of the ground state wave functions of the system, unlike other methods which to detect topological phases rely on non-local (string-like) operators [53, 144, 145, 146, 147], or nonlinear functions of the wave functions such as entanglement entropy and entanglement spectrum of the wave function [148, 149, 150], our approach is computationally more convenient. We also note that since we use ground states directly, this approach is also suitable for experimental data obtained from quantum simulators [151] and noisy intermediate-scale quantum (NISQ) devices [152].

4.1 Diffusion Map

The DMA is based upon the classical idea of integration that the global structure of a manifold can be determined by traversing it provided that local transition rules to move from one point to another is at hand. To do so, we create a Markov matrix of transitions for the points in the input data set, which guides a random walker to traverse the data set through a diffusion process which results in gaining information about the global geometrical properties of the input data. However, in order to probe the structure of the input data at different scales, a family of transition matrices are employed, and hence the name diffusion “maps”.

More concretely, suppose we have n input data, each represented by a N -dimensional vector $\vec{x}_\alpha = (x_\alpha^1, \dots, x_\alpha^N)$ in $\mathbb{R}^N$ where Greek letters denote the sample indices. For every two sampled vectors $\vec{x}_\alpha, \vec{x}_\beta$, we use the Euclidean metric to define their distance. To set the local rules of transition between two point we start by defining a symmetric positivity preserving function which for most applications could be a Gaussian kernel:

$$k(\vec{x}_\alpha, \vec{x}_\beta) = \exp\left(-\frac{|\vec{x}_\alpha - \vec{x}_\beta|^2}{\epsilon}\right), \quad (4.1)$$

where ϵ is the scaling hyperparameter of the DMA which determines the speed of the diffusion process of the corresponding random walker and correspondingly the number of clusters. We also define the diffusion matrix K which is a version of the graph Laplacian matrix with components $K_{\alpha\beta} = k(\vec{x}_\alpha, \vec{x}_\beta)$. To interpret this matrix as a probability distribution we need to normalize it by the diagonal matrix D whose components are

given by $D_{\alpha\alpha} = d_\alpha$ where $d_\alpha = \sum_\beta K_{\alpha\beta}$ and plays the role of the local degree of the graph. Then, the normalized Laplacian matrix is defined by

$$M = D^{-1}K, \quad (4.2)$$

Physically, the matrix M denotes the transition probabilities between different samples such that the probability of transition from sample α to β in t time steps is given by the t th power of this matrix i.e. $M_{\alpha\beta}^t$. We also notice that M is a stochastic matrix [153] with positive entries where each column sums to 1 and hence, the largest eigenvalue is 1. We should also notice that there are other choices for the distance function. One can change the L_2 norm to L_p norm for $p \geq 3$. As $p \rightarrow \infty$, we get the so-called Chebyshev's distance $d(\vec{x}_\alpha, \vec{x}_\beta) = \max_i |x_{\alpha i} - x_{\beta i}|$. One finds that in some cases, Chebyshev's distance may give sharper boundary condition [142]. We have tried other distance functions and our results for these distance functions are presented in the Appendix.

Next, we compute the diagonal representation of M . As in principal component analysis (PCA) where we only keep the largest eigenvalues to determine the number of clusters [154], here, we also keep the largest eigenvalues in the diagonal representation of M . We note that due to the spectral decay of the eigenvalues only a finite number of terms are necessary to achieve a given relative accuracy in reproducing M via its diagonal representation. Therefore, to reach an accuracy labeled by δ , we only need to keep the eigenvalues larger than $1 - \delta$ in the spectrum. Since δ is arbitrary, we can fix it, and then study how the number of relevant clusters vary with the scale parameter ϵ to probe the underlying geometric structure of the at different scales. We note that the main advantage

Hamiltonian H	parameters	Type of phase	ϵ	N
$-J' \sum_i \sigma_{2i-1}^- \sigma_{2i}^+ - J \sum_i \sigma_{2i}^- \sigma_{2i+1}^+ + h.c$	J, J'	Topological/Trivial	0.088	9
$\sum_i \cos(\theta) (\vec{S}_i \cdot \vec{S}_{i+1}) + \sin(\theta) (\vec{S}_i \cdot \vec{S}_{i+1})^2$	θ	H, Dimer, FM,	$\frac{1}{32}$	9
$\sum_i (\vec{S}_i \cdot \vec{S}_{i+1}) + B \sum_i S_x^i + \sum_i D (S_z^i)^2$	B, D	spin polarized, $\mathbb{Z}_2$ SB, H	$\frac{1}{32}$	10
$H = - \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - 2\Delta_s \sum_j c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \pm i\Delta_p/2 \sum_j (c_{j+1\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{j+1\downarrow} c_{j\uparrow}) + h.c.$	Δ_s, Δ_p	$N = 0, \pm 1$	$\frac{1}{32}$	6

Table 4.1: Summary of 1D Hamiltonians. H labels Haldane phase. Dimerized phase, Dimer phase, ferromagnetic phase, antiferromagnetic phase, XY phase, valence Bound state, $\mathbb{Z}_2$ symmetry breaking (SB) phase, critical phase.

of this method over more conventional ULMs such as PCA is that while maintaining the local structures of the data sets, it can also recognize their underlying nonlinear manifolds due to its nonlinear kernel which makes it advantageous compared to other unsupervised learning methods [155].

4.2 Model introduction and results

Let us now apply the DMA explained above to our quantum many-body problem. We imagine we are given a Hamiltonian with a set of unknown parameters $\theta \in \mathbb{R}^s$. We assume that we have direct access to the ground state of a N -particle many-body Hamiltonian and we can sample from its many-body wave function in the configuration space. In particular, in this study, for spin- σ chains our sampled wave function determines the configuration of the spins in the real space, and therefore, the components of the α 'th input vector are $x_\alpha^i = \{\pm\sigma\}$. For our fermionic and hard-core bosonic Hamiltonians, the measured wave function is represented in the Fock space, and therefore, $x_\alpha^i = \{0, 1\}$. In this setting, the schematic flowchart of our classification approach is illustrated in Fig.4.1, where $\psi_{\text{ground}}(\theta)$ denotes the ground state wave functions. In general, this state is a superposition of different product states. In the next step, the sampling is performed in the space of these product states resulting in the vectors $\vec{x}_\alpha(\theta)$ by which we can produce the

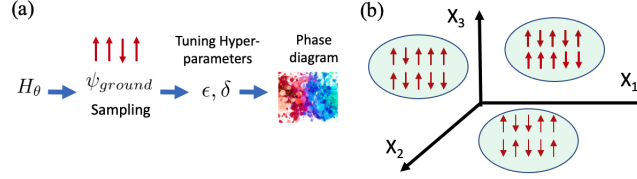


Figure 4.1: Schematic illustration of the machine-learning algorithms to identify different phases. (a) Flowchart of the diffusion maps algorithm. From a given Hamiltonian, (1) one obtains the ground state, and projectively samples from the ground state, (2) forms the diffusion matrix and tunes the hyperparameters, (3) obtains the phase diagram by finding the conspicuous transitions in the number of eigenvalues. (b) Different ground states in a cluster can transform to each other via a diffusion process in the dataset basis.

corresponding Laplacian matrix $M(\theta)$. Since, across quantum phase transitions usually a change in the relevant degrees of freedom that describe the system occurs, we expect that for a given accuracy δ , once the scale ϵ is chosen properly, the number of clusters obtained from $M(\theta)$ should reveal the underlying phase diagram of the system.

To determine the proper regime for ϵ as the parameter that describes the dynamics of the diffusion process [137], we use the approximate analysis of the spectrum of M proposed in [138, 139]. Assuming clusters of samples with r particles in different configuration states, the diffusion matrix K will acquire a block-diagonal form with each block corresponding to a single such clusters. In this representation, diagonal elements are close to the identity while off-diagonal components are bounded by $\mathcal{O}(e^{-r/\epsilon})$. Denoting the number of such clusters with N_c , after diagonalizing K , we will approximately have N_c eigenvalues larger than $1 - e^{-r/\epsilon}$ and therefore the accuracy can be approximated by $\delta \sim e^{-r/\epsilon}$. Thus by choosing $\epsilon \sim -r/\ln\delta$, we can find the number of clusters of a particular size r . Consequently, since the number of particles in the clusters can change between 1 to N , we need to span the corresponding range of ϵ , to obtain the best value of ϵ empirically where changes in N_c show a conspicuous change for different values of θ .

Therefore, sharp changes in N_c as a function of θ can be presumed to trace the topological phase transitions.

In what follows we employ the procedure above, and consider some of the most well-known models which describe SPT phases and we demonstrate that we can reproduce their phase diagram with an acceptable precision. We summarize our models in table 4.1 where for all models we have $\delta = 0.00001$) and we use periodic boundary conditions. For all of these models we generate the many-body ground state of the system in the Fock space and then sample from the states that their superposition creates the ground state of the system. We collect 500 samples for each fixed parameters in the Hamiltonian.

Model 1: Nontrivial SPT/Symmetry-protected trivial.— In this section, we ask whether we can distinguish between ground states with a trivial phase and a non trivial SPT phase [151]. As one of the simplest models, we start with the interacting version of the SSH model which has been recently realized via Rydberg atoms and describes a topological phase transition between a SPT non-trivial and trivial phase. This model can be described by hard-core bosons $b_i^2 = 0 = b_i^{\dagger 2}$. We consider two alternating coupling constants denoted by J and J' between adjacent sites $(n, n+1)$, where the former couples sites with odd n , and the latter couples sites with even n ,

$$H_{J,J'} = \sum_{ij} J_{ij} (b_i b_j^\dagger + b_j b_i^\dagger), \quad (4.3)$$

As shown in [151] this model is mapped to the fermionic SHH model whose energy spectrum consists of two bands separated by a spectral gap $2(|J| - |J'|)$. Most importantly,

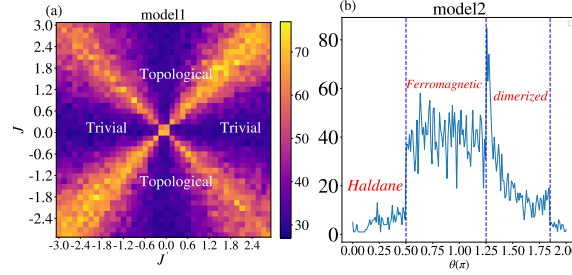


Figure 4.2: Phase diagrams of model 1 and 2. Colorbar in (a) and vertical axis in (b) represent the number of eigenvalues larger than $1 - \delta$ (See text). (a) Model 1 is an interacting bosonic SPT model with a topological and trivial phase with phase boundaries at $J = \pm J'$. (b) Model 2 is biquadratic spin chain model whose ground state at $\theta = 1/3$ is the AKLT state. The dashed lines illustrate the phase boundaries obtained via DMRG methods.

this model for $|J'| > |J|$ is a topologically trivial phase while for $|J'| < |J|$ it becomes a topological SPT phase which with open boundary conditions hosts delocalized zero-energy edge modes. In this case, the symmetry group $G = \mathbb{Z}_2 \times \mathbb{Z}_2$ based on group cohomology classification only has one non-trivial topological phase since $H^2[\mathbb{Z}_2 \times \mathbb{Z}_2; U(1)] = \mathbb{Z}_2$. Using Jordan-Wigner transformation, the original representation of this model transforms into a spin chain Hamiltonian [151]:

$$H = -J' \sum_i \sigma_{2i-1}^- \sigma_{2i}^+ - J \sum_i \sigma_{2i}^- \sigma_{2i+1}^+ + h.c. \quad (4.4)$$

We use the natural spin basis as our sampling result. We can see in Fig. 4.2(a) that our method reproduces the phase diagram obtained in [151].

Model 2: AKLT.— Here, compared to model 1, as a more challenging situation, we ask whether our approach can detect SPT phases with more involved symmetries where symmetry broken phases may exist, too. The Haldane phase of $S = 1$ antiferromagnetic spin chains is a well-known example of such SPT phases with a $\mathbb{Z}_2 \times \mathbb{Z}_2$

symmetry group whose parent Hamiltonian can host several symmetry broken phases. An example of states in the Haldane phase which can be written in a closed form, is the AKLT state [156]. This state is a special case of the ground state of the following bilinear-biquadratic spin-1 Hamiltonian ($\vec{S}_i$ are spin-1 operators) when $\theta = 1/3$,

$$H_{\text{bb}} = \sum_i \cos(\theta_{\text{bb}})(\vec{S}_i \cdot \vec{S}_{i+1}) + \sin(\theta_{\text{bb}})(\vec{S}_i \cdot \vec{S}_{i+1})^2. \quad (4.5)$$

However, by varying θ this model describes two topological and non-topological phase transitions.

We can apply the DMA to this model with $N = 9$ and plot the resulting phase diagram Fig. 4.2(b) which is akin to the results in [106]. Here, we again see another successful detection of an SPT phase where two additional symmetry broken phases may compete with each other.

Model 3: Variants of AKLT.— As an another more complicated model, we study a variant of the *AKLT* model where in addition to symmetry broken and topological phases we also have a time reversal invariant (TRI) phase with the same symmetries as the Haldane phase [157],

$$H = \sum_i (\vec{S}_i \cdot \vec{S}_{i+1}) + B \sum_i S_x^i + \sum_i D(S_z^i)^2. \quad (4.6)$$

This Hamiltonian is invariant under translational symmetry, $\mathbb{Z}_2$ time reversal symmetry $S_y \rightarrow -S_y$ and $\mathbb{Z}_2$ parity symmetry. The complete description of the phase diagram is found in [157] which contains a time reversal invariant (TRI) phase with

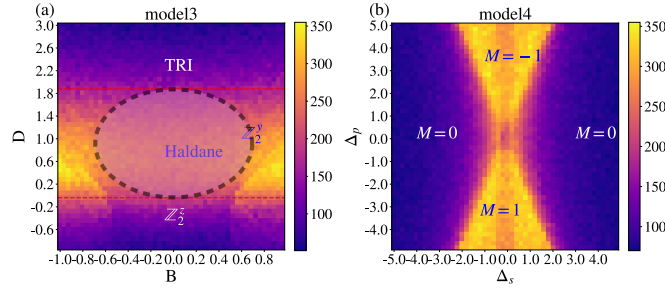


Figure 4.3: Phase diagrams of model 3 and model 4. (a) Model 3 is a variant of the AKLT model which hosts one trivial phase (TRI), two symmetry breaking phases ($\mathbb{Z}_2^y$, and $\mathbb{Z}_2^x$), and one topologically ordered phase (Haldane). The topological classification of the system is described by the $\mathbb{Z}_2$ group. The dashed line shows the approximate boundaries of the Haldane phase obtained via exact methods. (b) Model 4 is a weakly interacting fermionic model with unconventional pairing. C labels the states via their distinct zero modes in different phases which is obtained via exact diagonalization. Colorbars represent the number of eigenvalues larger than $1 - \delta$ (See text).

$S^z = 0$, and two symmetry broken phases, $\mathbb{Z}_2^{x,y}$, and the Haldane phase. Our results for this model is depicted in Fig. 4.3(a). In this figure by comparing our phase diagram with those obtained in [157], we can see a noticeable transition between the $\mathbb{Z}_2^x$, TRI and the Haldane phase. However, the distinction between the $\mathbb{Z}_2^y$ and the Haldane phase is less pronounced and we only see a partial change of color between these two regions.

Model 4.— In models 1 – 3 based on group cohomology arguments the topological classification of the phases is described by the $\mathbb{Z}_2$ group, and there is only one topologically non-trivial phase. Here, in addition to spin-1 chains, we consider a *weakly* interacting fermionic spin-1/2 Hamiltonian which can host more than one non-trivial SPT phase whose topological classification is described by the $\mathbb{Z}_2 \times \mathbb{Z}_2$ group. This model respects both time reversal symmetry and S_z spin-rotation symmetries. Hence, in the absence of interactions, based on the 10-fold classification, its topological phases are

described by the $\mathbb{Z}$ group. Nevertheless, by adding interactions to this Hamiltonian, the resulting topological classes of this system will reduce to the $\mathbb{Z}_2 \times \mathbb{Z}_2$ group. The BdG form of this Hamiltonian is given by, [158]:

$$H = - \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - 2\Delta_s \sum_j c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \\ \pm i\Delta_p/2 \sum_j (c_{j+1\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{j+1\downarrow} c_{j\uparrow}) + \text{h.c.},$$

where the last term is an unconventional pairing between electrons on adjacent sites. This model, can host three phases labeled by $M = 0, +1, -1$, which represents the states with distinct zero modes ¹. We simulate this model with $N = 6$, and plot the resulting phase diagram in Fig. 4.3(b).

As we can in this figure, our approach can regenerate the phase diagram of this model as obtained in [158] with a high accuracy. To be more specific, we see sharp transitions between the topologically non-trivial phases with $M = \pm 1$ and trivial phases labeled by $M = 0$. While in principle, from this plot we cannot distinguish the $M = \pm 1$ phases from each other, from the fact that we see a conspicuous change in the number of eigenvalues at their intersection at $\Delta_{s,p} \simeq 0$ we may speculate that the two regions correspond to distinct phases. This indicates that DMA not only can differentiate between topologically trivial phases and topologically non-trivial phases, but also can provide evidence for differentiating between different topological phases with similar properties.

Discussion and Outlook.—

¹As demonstrated in [158] by stacking two chains with $C = +1$, we get another non-trivial phase with two zero modes. In the presence of strong interactions the phase with $C = -1$ and $C = 3$ are identified and hence the classification is $\mathbb{Z}_4$.

In this work, we have used an unsupervised learning algorithm called diffusion maps to detect topological phase transitions between different symmetry broken phases and different SPT phases. Our results demonstrate that using diffusion maps as a computationally inexpensive method, can provide helpful evidence for the presence of SPT phase transitions and SPT phases. Since previously this algorithm has been used for detecting other symmetry broken phase transitions in one dimension [138], and due to the lack of intrinsic topological order in one dimension, our results demonstrate that the DMA can detect all different types of equilibrium phase transitions in one dimension.

From a conceptual viewpoint, the reason behind the efficacy of the DMA in detecting SPT phases is thought-provoking. One possible explanation is that the DMA in the continuum limit approximates the differential heat equation. On the other hand, the spectrum of elliptic differential operators such as the heat kernel appearing in the heat equation, can include important information about topological invariants [159, 160]. Based on our results, we speculate that these conceptual relations between the spectrum of differential operators and SPT invariants have practical application for computational and experimental purposes.

An immediate question to be pursued in future is the detection of SPT phases in higher dimensions via the DMA. Another intriguing question to investigate, is the detection of long-range topological order in symmetry enriched topological phases [161] which can be realized in two and higher dimensions without using thermal sampling [141]. Also, detection of topological phases in non-equilibrium phases of matter especially Floquet systems is left for future studies.

In this supplemental, we consider two additional spin chain models which can host

SPT phases. We consider the following Hamiltonian with periodic boundary condition as considered for other models in the main text, [162]:

$$H = \sum_i S_x^i S_x^{i+1} + S_y^i S_y^{i+1} + \lambda S_z^i S_z^{i+1} + D(S_z^i)^2. \quad (4.7)$$

We can use the same techniques and with $L = 9$ and 2500 samples to implement the diffusion map algorithm (DMA) by using Euclidean distance and Chebyshev's distance. We can see sharper phase boundary condition by using Chebyshev's distance. We use L_2 and L_∞ to denote them, respectively. We plot the phase diagram via the DMA. The phase diagram Fig. 4.4 matches with the predictions in [162] to a great extent. In particular the distinction between the antiferromagnetic phase (AFM), Haldane and the ferromagnetic phases are completely distinguishable, however, we observe a less evident transition between the Haldane and the dimerized phases. We also notice that we have not detected the XY phase whose presence is still undetermined via exact methods [162].

The second model that we consider here is the following spin Hamiltonian with periodic boundary condition [162]:

$$H = \sum_i J_i (S_i \cdot S_{i+1} - \beta (S_i \cdot S_{i+1})^2). \quad (4.8)$$

$J_i = 1$ for i even, $J_i = \omega$ for i is odd. We can see our method Fig. 4.5 matches qualitatively with [162] and we can see a sharp transition between the topological Haldane phase and two symmetry broken phases i.e. valence bond state (VBS) and dimerized phases. We can also predict $\beta = -\frac{1}{3}$ [162] for the transition from VBS to Haldane phase.

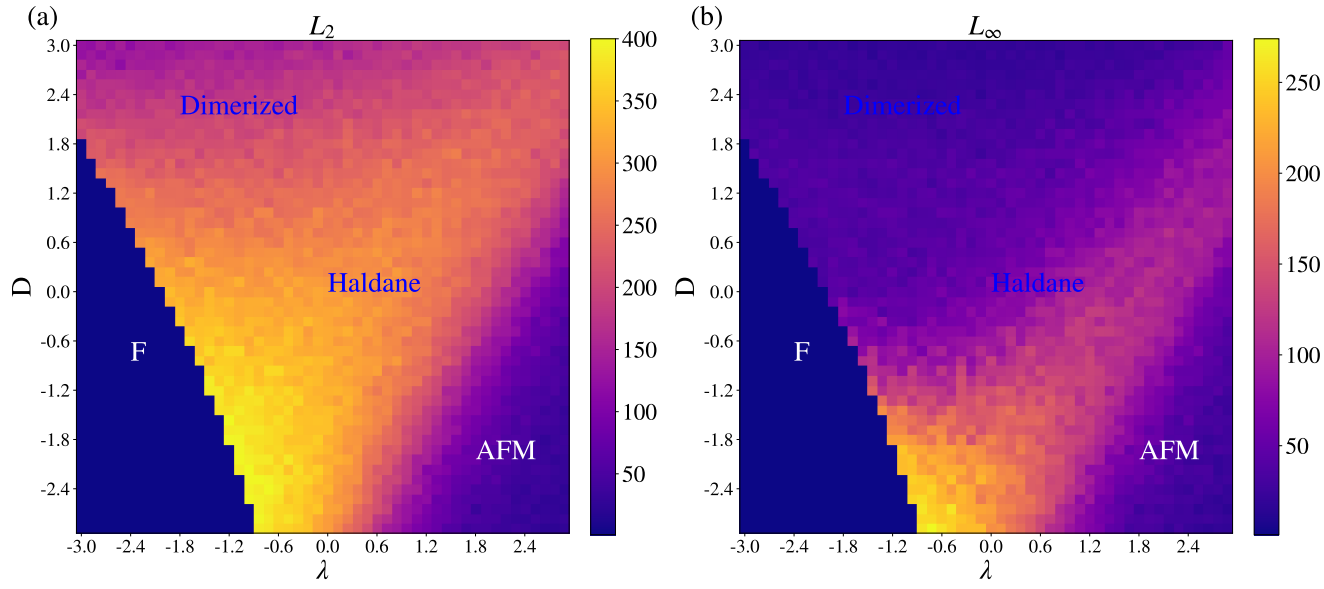


Figure 4.4: Phase diagram of Hamiltonian in Eq.4.7 in terms of λ, D obtained via the diffusion maps algorithm. Dashed lines represent the exact phase boundaries obtained by DMRG methods.

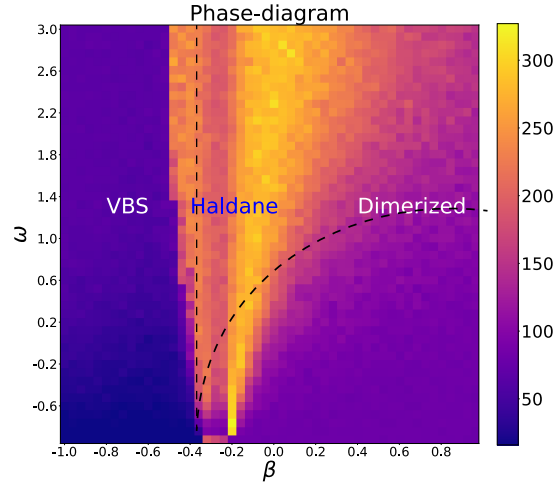


Figure 4.5: Phase diagram of Hamiltonian in Eq.4.8 in terms of β, ω obtained via the diffusion maps algorithm. Dashed lines represent the exact phase boundaries obtained by DMRG methods.

4.3 PCA and k-means algorithm

To compare the performance of the diffusion maps algorithm and other unsupervised methods, here, we try one of the most standard unsupervised algorithm called PCA (principle component analysis) on our sampling and compute the mean of 2 components. After doing this, we choose the number of clusters and use the standard k means algorithm. It should be highlighted that we do not have to pick the number of clusters in the diffusion map algorithm. We choose model 3 [157] in our main text.

$$H = \sum_i (\vec{S}_i \cdot \vec{S}_{i+1}) + B \sum_i S_x^i + \sum_i D(S_z^i)^2. \quad (4.9)$$

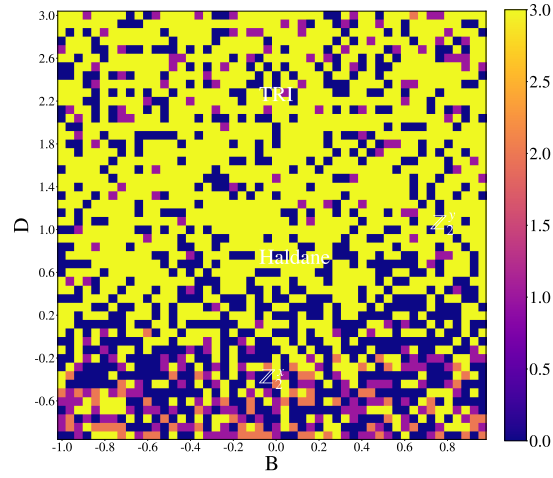


Figure 4.6: PCA and k means on model 3

Here, we find that this method fails to identify the phase transition in fig 4.6 completely.

This superior performance of the diffusion maps in comparison to other unsupervised learning methods is due to the fact that in this approach we use non-linear kernel functions which allow us to detect complicated non-linear structures in data sets.

Chapter 5: Conclusion and Outlook

In this dissertation, we first describe the generalized boson sampling which can be viewed as a completely new hypothetical quantum supremacy experiment by modifying the original proposal of [5]. We also considered machine learning applications in scientific discovery, especially in the phase transition involving the conformal field theory [127] and symmetric protected topological phases [163].

In chapter 2, One open question in quantum supremacy is how to verify that a quantum computer has indeed achieved quantum supremacy. This involves demonstrating that the quantum computer can solve a problem that would be infeasible for a classical computer and that the solution produced is correct. This is tightly related to so-called interactive proof in computational complexity. Three famous examples including $IP = PSPACE$ [164], $MIP = NEXP$ [165], $MIP^* = RE$ [166]. Now suppose Merlin has only BQP power instead of PSPACE power, can Merlin show this fact to Arthur? Another open question is whether quantum supremacy will have practical implications beyond demonstrating the potential of quantum computers. While achieving quantum supremacy is a significant milestone in the development of quantum computing, it is not yet clear what specific applications will benefit from this capability. There are also open questions related to the scalability and robustness of quantum computing technology,

as well as the development of quantum algorithms and software that can effectively utilize quantum hardware. Additionally, there are questions about the potential impact of quantum computing on cryptography and information security [167, 168]. Finally, we can also talk about what kind of problems NISQ can solve. NISQ devices [152, 169] stands for "Noisy Intermediate-Scale Quantum" and refers to a type of quantum computer that is currently available and has a limited number of qubits (quantum bits) and a high level of noise and errors in its operations. These types of quantum computers are considered to be intermediate in terms of their capabilities and are not yet able to perform large-scale, error-corrected quantum computations. However, NISQ devices can still be useful for certain types of quantum algorithms and simulations, as well as for exploring the potential of quantum computing. Standard NISQ platform including superconducting qubit [170, 171, 172], trapped ions [173], and Rydberg atoms [174].

In the rest of the thesis, we discuss two machine learning applications on quantum systems especially focusing on phase transition. This type of machine learning and interaction with quantum is often referred to as CQ. Quantum machine learning is a rapidly growing field that combines quantum computing and classical machine learning techniques. There are generally four different areas in quantum machine learning and each has its own open questions. Our thesis only covers a tiny island in such a profound area. We summarize them in the following:

1. Quantum algorithms for machine learning [175]: Quantum algorithms for machine learning is a rapidly developing field that explores the use of quantum computers to speed up traditional machine learning algorithms. One open question in this

area is how to design quantum machine learning algorithms that are both efficient and effective. Currently, most quantum machine learning algorithms are designed to solve specific problems or make specific predictions, rather than being general-purpose algorithms that can be applied to a wide range of problems. As such, one open question is how to develop more general quantum machine learning algorithms that can be used to solve a wide range of problems. Another open question is how to effectively train and optimize quantum machine learning algorithms. Unlike classical machine learning algorithms, quantum machine learning algorithms can be challenging to train due to the complexity of the quantum hardware and the need for specialized knowledge of quantum mechanics. Additionally, there is a need for new techniques to validate and test quantum machine learning algorithms, as traditional methods may not be appropriate for quantum systems. Finally, there is also the question of how to integrate quantum machine learning algorithms with existing classical machine learning tools and frameworks.

2. Quantum-inspired classical algorithms [176]: This area focuses on using ideas from quantum computing to develop new classical machine learning algorithms. One example is the quantum-inspired kernel method [177, 178, 178, 179], which uses quantum algorithms to efficiently calculate kernel functions in classical machine learning algorithms.
3. Quantum data encoding: This area focuses on encoding classical data into quantum states in order to take advantage of quantum algorithms. One example is the

quantum principal component analysis algorithm [180], which can extract principal components from a quantum-encoded dataset.

4. Quantum hardware for machine learning: This area focuses on developing quantum hardware that is specifically designed for machine learning tasks. For example, quantum annealers [181] which is a computational method that seeks to solve optimization problems by using quantum mechanics. The idea is to use a quantum system to explore the search space of a problem and find the solution that minimizes the objective function. One open problem in quantum annealing is the so-called "quantum speedup" problem. While quantum annealing has shown promise in solving certain optimization problems, it is still not clear whether it can provide a significant speedup over classical methods for all types of optimization problems [182]. Another open problem is the optimization of the annealing schedule [183, 184], which determines the rate at which the system transitions from its initial state to the final state. There is currently no consensus on the best way to optimize the annealing schedule, and different schedules may be optimal for different problems. Finally, there is the issue of quantum coherence and noise in quantum annealing systems. Quantum coherence [185] is essential for the success of quantum annealing, but it is also very fragile and can be easily disrupted by external noise. Developing better error-correction techniques and noise-resistant hardware is an ongoing challenge in the field.

Appendix A:

A.1 Generalized Bosons

In this section, we introduce the definition of generalized boson. In the next section, we will then show that FBS will still yield a permanent when sampling from the output distribution of linear mode mixing applied to generalized Fock states.

To define generalized bosons, first, recall the definition of a standard boson from regular quantum field theory [186]. Let A be a nonempty set. We can associate each $i \in A$ with a pair of operators $a_i, a_i^\dagger$, corresponding to annihilating and creating a boson, respectively. Those operators satisfy the following commutation relations

$$[a_i, a_j^\dagger] \equiv a_i a_j^\dagger - a_j^\dagger a_i = \delta_{ij}, \quad [a_i^\dagger, a_j^\dagger] = [a_i, a_j] = 0, \quad (\text{A.1})$$

where δ_{ij} is the Kronecker delta.

For generalized bosons, we proceed analogously, except that we relax the diagonal commutation relation requirement in the following sense

$$[b_i, b_j^\dagger] = \delta_{i,j} \sum_{n_i=0}^{\infty} F(n_i) |n_i\rangle \langle n_i|, \quad [b_i^\dagger, b_j^\dagger] = [b_i, b_j] = 0, \quad (\text{A.2})$$

where $F : \mathbb{N}_0 \rightarrow \mathbb{C}$ may be an arbitrary complex-valued scalar function. We recover the definition of standard bosons by defining $F(n) \equiv 1, \forall n \in \mathbb{N}_0$, which corresponds to the identity operator.

We define the generalized Fock basis by the action of the generalized bosonic creation operator on the vacuum state as

$$(b^\dagger)^n |0\rangle = f(n) |n\rangle, \quad (\text{A.3})$$

where $f : \mathbb{N}_0 \rightarrow \mathbb{C}$ is an alternative characterization of a generalized boson that is equivalent to F . For $n = 0$, we always have $f(0) = 1$ due to Eq. (A.3).

To see this, let us first show how F is determined by f . To this end, observe the following standard relation for the action of a creation and annihilation operator on a Fock state $|n\rangle$

$$b^\dagger |n\rangle = \frac{f(n+1)}{f(n)} |n+1\rangle, \quad b |n\rangle = \frac{f(n)}{f(n-1)} |n-1\rangle. \quad (\text{A.4})$$

Given this, we can compute

$$F(n) = \langle n | [b, b^\dagger] | n \rangle = \frac{f(n+1)^2}{f(n)^2} - \frac{f(n)^2}{f(n-1)^2}. \quad (\text{A.5})$$

Conversely, we can construct f given F recursively via the following relation

$$\frac{f^2(n+1)}{f^2(n)} = \frac{f(1)^2}{f(0)^2} + \sum_{i=1}^n F(i). \forall n \geq 1, \quad (\text{A.6})$$

and the requirement of $f(0) = 1$ as well as the observation that $\frac{f(1)^2}{f(0)^2} = F(0)$ so that

$f(1) = \sqrt{F(0)}$. So once we fixed $F(i) \forall i \in \mathbb{N}$ and $f(0) = 1$, f is recursively determined by Eq. (A.6). In particular, if we choose $F(i) = 1, \forall i$ we obtain $f(n) = \sqrt{n!}$ as we would expect.

So the bosonic factor completely determines all the structure of generalized bosons and vice versa. We will see how the order structure of $f(n)$ will play an important rule in our context.

We can then define the multimode Fock state of generalized bosons in M modes as

$$|n_1, n_2, \dots, n_M\rangle = \left(\prod_{i=1}^M \frac{1}{f(n_i)} \right) b_1^{\dagger n_1} b_2^{\dagger n_2} \dots b_M^{\dagger n_M} |0\rangle^M. \quad (\text{A.7})$$

A.2 Bosons sampling with generalized bosons

We now derive FBS for generalized boson and show its output probability is still proportional to a permanent of mode-mixing matrix Λ .

Theorem A.2.1. *Consider a linear transformation $\Lambda \in U(M)$ of M modes of a generalized bosonic algebra on those modes with bosonic factor f . Then the probability of measuring outcome $\mathbf{k}$ given a Fock input state $|\mathbf{l}\rangle$ is given by*

$$\text{Pr}(\mathbf{k}|\mathbf{l}) = \left(\prod_{i=1}^M \frac{f(k_i)}{f(l_i)k_i!} \right)^2 |\text{Perm}(\Lambda[\mathbf{k}|\mathbf{l}])|^2. \quad (\text{A.8})$$

where $\Lambda[\mathbf{m}|\mathbf{n}]$ is an $(N \times N)$ matrix constructed by repeating the i^{th} column of Λ l_i many times, and the j^{th} row k_i many times. We start the proof: The unitary transformation

Λ acts like the following:

$$\mathbf{b} \rightarrow \Lambda^\dagger \mathbf{b}, \mathbf{b}^\dagger \rightarrow \Lambda^T \mathbf{b}. \quad (\text{A.9})$$

We can expand the $\Lambda^\dagger \mathbf{b}$ by using multinomial expansion theorem (to use multinomial expansion, we must only require $[b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0$). We first compute Λ acting on the input state $|\mathbf{l}\rangle = |l_1, l_2, \dots, l_M\rangle$. We have

$$\Lambda |l_1, l_2, \dots, l_M\rangle = \quad (\text{A.10})$$

$$\prod_{i=1}^M \frac{1}{f(l_i)} \sum_{\{n_{ij}, \sum_{j=1}^M n_{ij}=l_i\}} \frac{l_i!}{\prod_{i,j=1}^M n_{ij}!} \left(\prod_{j_1=1}^M \Lambda_{j_1 1} b_{j_1}^\dagger \right)^{n_{1j_1}} \left(\prod_{j_2=1}^M \Lambda_{j_2 2} b_{j_2}^\dagger \right)^{n_{2j_2}} \dots \left(\prod_{j_M=1}^M \Lambda_{j_M M} b_{j_M}^\dagger \right)^{n_{Mj_M}} |0\rangle^M. \quad (\text{A.11})$$

$$= \sum_{\sum_{j=1}^M k_j = N} C_{\mathbf{k}|\mathbf{l}} |\mathbf{k}\rangle,$$

where the coefficient $C_{\mathbf{k}|\mathbf{l}}$ is given by

$$C_{\mathbf{k}|\mathbf{l}} = \prod_{i=1}^M \frac{l_i!}{f(l_i)} \prod_{j=1}^M f(k_j) \sum_{\{n_{ij}: \sum_{j=1}^M n_{ij}=l_i, \sum_{i=1}^M n_{ij}=k_j\}} \frac{\prod_{i,j=1}^M \Lambda_{ji}^{n_{ij}}}{\prod_{i,j=1}^M n_{ij}!}. \quad (\text{A.12})$$

We use the following combinatorial identity [5, 23]

$$\sum_{\{n_{ij} \in \mathbb{N}_0: \sum_{j=1}^M n_{ij}=l_i, \sum_{i=1}^M n_{ij}=k_j\}} \frac{\prod_{i,j=1}^M \Lambda_{ji}^{n_{ij}}}{\prod_{i,j=1}^M n_{ij}!} = \left(\prod_{i=1}^M \frac{1}{l_i!} \right) \left(\prod_{j=1}^M \frac{1}{k_j!} \right) \text{Perm}(\Lambda[\mathbf{k}|\mathbf{l}]). \quad (\text{A.13})$$

Finally, we get (notice that $f(0) = 1$):

$$C_{\mathbf{k}|\mathbf{l}} = \left(\prod_{i=1}^N \frac{f(k_i)}{f(l_i)k_i!} \right) |\text{Perm}(\Lambda[\mathbf{k}|\mathbf{l}])|. \quad (\text{A.14})$$

which finishes the proof as $\Pr(\mathbf{k}|\mathbf{l}) = |C_{\mathbf{k}|\mathbf{l}}|^2$ which finishes the proof.

In particular, when we choose the standard-bosonic $f(n) = \sqrt{n!}$, (A.14) reduces to the output probabilities of standard FBS

$$\Pr(\mathbf{k}|\mathbf{l}) = \frac{|\text{Perm}(\Lambda[\mathbf{k}|\mathbf{l}])|^2}{(\prod_i l_i!) (\prod_i k_i!)}. \quad (\text{A.15})$$

which recovers the result of FBS [5, 23].

Since the prefactors of the probabilities will always be a constant in the collision-free subspace, i.e., whenever $k_i, l_i \in \{0, 1\}$, the hardness results of [5] directly apply to generalized boson sampling.

A.3 Gaussian Boson Sampling for Generalized Boson

In this section, we generalize the Gaussian-state formalism to generalized bosons. As it turns out, key features of this formalism do not generalize, making it somewhat contrived. Nonetheless, it can be used to show that the outcome probability of the analogue of GBS are also given by Hafnians.

To begin with, we introduce the definition of a coherent state, central to the Gaussian formalism, in Sec. A.3.1. We then derive the P and Q function in Sec. A.3.2 and use it to compute the outcome probabilities of generalized GBS in Sec. A.3.4.

A.3.1 Generalized Coherent States

In this section, we introduce the coherent state of generalized bosons. We define

$|\alpha\rangle = \frac{1}{\sqrt{N(\alpha)}} e^{\alpha a^\dagger} |0\rangle$ for a generalized bosonic operator a with bosonic factor f as

$$|\alpha\rangle = \frac{1}{\sqrt{N(\alpha)}} \sum_{n=0}^{\infty} \frac{(\alpha a^\dagger)^n}{n!} |0\rangle = \frac{1}{\sqrt{N(\alpha)}} \sum_{n=0}^{\infty} \frac{(\alpha)^n}{n!} f(n) |n\rangle, \quad (\text{A.16})$$

where $N(\alpha)$ is a normalization factor that enforces $\langle\alpha|\alpha\rangle = 1$, as given by

$$N(\alpha) = \sum_{n=0}^{\infty} \frac{|\alpha|^{2n} f^2(n)}{n!^2}. \quad (\text{A.17})$$

We can then compute the inner product of two generalized coherent states $\langle\beta|$ and $|\alpha\rangle$ as

$$\langle\beta|\alpha\rangle = \frac{1}{\sqrt{N(\alpha)N(\beta)}} \sum_{n=0}^{\infty} \frac{(\beta^* \alpha)^{2n} f^2(n)}{n!^2}. \quad (\text{A.18})$$

Indeed, if we choose the bosonic factor to be $f(n) = \sqrt{n!}$, then we obtain $N(\alpha) = e^{|\alpha|^2}$,

which reproduces the standard coherent state

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle = e^{-\frac{|\alpha|^2}{2}} e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} |0\rangle. \quad (\text{A.19})$$

A.3.2 P and Q Functions for Generalized Boson

Phase space methods are widely used in quantum optics. The advantage of phase space methods is that in order to compute an expectation value of an observable, one only

needs to compute an integral over phase space instead of calculating a trace. Specifically, the P and Q functions are the most widely used representations of observables and density matrices in phase space [187, 188], respectively.

In this section, we define the P and Q functions for generalized bosons. Before we start studying the P and Q functions, we need to first figure out the normalization constant of the generalized coherent basis. In the single mode case, we have the integral

$$\int |\alpha\rangle \langle\alpha| d^2\alpha = \kappa I. \quad (\text{A.20})$$

where κ is a positive constant. For example, for the q -boson coherent state, we have $\kappa = \pi$, and for the spin coherent state, we have $\kappa = \frac{4\pi}{2S+1}$. The expectation of an operator O can then be written as an integral over a two-dimensional phase space with coordinates α, α^* :

$$\text{tr}[\rho O] = \int d^2\alpha \frac{1}{\kappa} \langle\alpha| \rho O |\alpha\rangle. \quad (\text{A.21})$$

We use this expression in order to define the phase space representation of a density matrix ρ , named Q -function, as $Q_\rho(\alpha) = \frac{1}{\kappa} \langle\alpha| \rho |\alpha\rangle$ where the κ^{-1} factor serves to ensure that the Q -function is normalized in the sense of

$$\int Q_\rho(\alpha) d^2\alpha = 1 \quad \& \quad (\text{A.22})$$

Intuitively, we can think of the Q -function as the projection of the density matrix ρ onto the coherent-state basis. In the M -mode case, the Q -function is then given by $Q_\rho(\boldsymbol{\alpha}) = \kappa^{-M} \langle\boldsymbol{\alpha}| \rho |\boldsymbol{\alpha}\rangle$, where $|\boldsymbol{\alpha}\rangle = |\alpha_1\rangle \otimes \cdots \otimes |\alpha_M\rangle$.

Since the Q -function is the phase space representation of a density matrix ρ , similarly, we also map the observable to its corresponding phase space representation namely the P -function. For the purpose of this work, we only need observables which are projective measurements in the Fock basis. The P -function of a single-mode projective Fock measurement $|n\rangle \langle n|$ is defined as the function $P_n : \mathbb{C} \rightarrow \mathbb{R}$ which satisfies

$$|n\rangle \langle n| = \int d^2\alpha |\alpha\rangle \langle \alpha| P_n(\alpha). \quad (\text{A.23})$$

For the multi-mode case, the P -function P_n is defined by the analogous relation $|\mathbf{n}\rangle \langle \mathbf{n}| = \int d^{2M}\alpha |\boldsymbol{\alpha}\rangle \langle \boldsymbol{\alpha}| P_n(\boldsymbol{\alpha})$.

Given those definitions, we can write the probability of measuring a multi-mode Fock state $|\mathbf{n}\rangle = |n_1, n_2, \dots, n_N\rangle$ on a density matrix ρ as

$$\text{Pr}(\mathbf{n}) = \int d^{2M}\alpha Q_\rho(\boldsymbol{\alpha}) P_n(\boldsymbol{\alpha}). \quad (\text{A.24})$$

For generalized bosons, the Q -function can be obtained straightforwardly while the P -function is nontrivial. Since $|\mathbf{n}\rangle = |n_1\rangle \otimes \dots \otimes |n_N\rangle$ is a product state, its P -function is a product of single-mode P -functions acting on each mode individually. This can be seen by generalizing Eq. (A.26) to multi-mode Fock states. It turns out that the single-mode P -function for $|n\rangle \langle n|$ can be written as

$$P_n(\alpha) = N(\alpha) \frac{1}{f(n)^2} \left(\frac{\partial^2}{\partial \alpha \partial \alpha^*} \right)^n \delta(\alpha) \delta(\alpha^*). \quad (\text{A.25})$$

To see this, let us verify it by the definition of P -function. by integrating $P_n(\alpha)$ over

phase space

$$\begin{aligned}
\int d^2\alpha |\alpha\rangle \langle\alpha| P_n(\alpha) &= \int d^2\alpha |\alpha\rangle \langle\alpha| N(\alpha) \frac{1}{f(n)^2} \left(\frac{\partial^2}{\partial\alpha\partial\alpha^*} \right)^n \delta(\alpha)\delta(\alpha^*) \\
&= \frac{1}{f(n)^2} \int d^2\alpha \sum_{k,l=0}^{\infty} \frac{\alpha^k \alpha^{*l}}{k!l!} f(k)f(l) |k\rangle \langle l| \left(\frac{\partial^2}{\partial\alpha\partial\alpha^*} \right)^n \delta(\alpha)\delta(\alpha^*) \\
&= \frac{1}{f(n)^2} \int d^2\alpha \delta(\alpha)\delta(\alpha^*) \left(\frac{\partial^2}{\partial\alpha\partial\alpha^*} \right)^n \sum_{k,l=0}^{\infty} \frac{\alpha^k \alpha^{*l}}{k!l!} f(k)f(l) |k\rangle \langle l| \\
&= |n\rangle \langle n|.
\end{aligned} \tag{A.26}$$

Here, we use the property of the delta function, since once we take the partial derivative $\left(\frac{\partial^2}{\partial\alpha\partial\alpha^*} \right)^n$ inside integral, only the $|n\rangle$ component remains after integration. Because the delta function eliminates all the terms depending on α after partial derivatives, $|n\rangle$ is the only component that does not depend on α after we take the partial derivative.

The P -function of a multi-mode Fock state $|n\rangle$ is then given by

$$P_n(\alpha) = \frac{1}{\prod_{i=1}^M f(n_i)^2} e^{\sum_{i=1}^M \ln(N(\alpha_i))} \prod_{j=1}^M \left(\frac{\partial^2}{\partial\alpha_j\partial\alpha_j^*} \right)^{n_j} \delta(\alpha_j)\delta(\alpha_j^*). \tag{A.27}$$

A.3.3 Generalized Gaussian states

Given the phase-space representation in terms of the P and Q function, we define a Gaussian state for generalized bosons analogously to the standard case, if it has a Gaussian Q -function in the sense that

$$Q_\rho(\alpha) = \frac{1}{g\sqrt{|\sigma_Q|}} e^{-\frac{1}{2}\alpha^\dagger \sigma_Q^{-1} \alpha} \tag{A.28}$$

for some positive semidefinite matrix σ_Q , called the covariance matrix. Here, $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_M)^T$, $\alpha^\dagger = (\alpha_1^*, \alpha_2^*, \dots, \alpha_M^*)$, $|\sigma_Q|$ is the determinant of σ_Q , and g is a normalization constant which makes $\int Q(\alpha) d^{2M} \alpha = 1$ with $d^{2M} \alpha = \prod_{i=1}^M d^2 \alpha_i$.

Let us point out, however, that Gaussian states are highly unnatural for generalized bosons. Let us elaborate this point: Generally speaking, given a basis, one can define a Gaussian state in the Q representation for generalized bosons. Here, we did so by introducing a generalized coherent state, and defining the Q -function in the generalized coherent state basis. However, in contrast to the standard boson, the displacement operator will not prepare a Gaussian state, and neither will the squeezing operator prepare a Gaussian state. Hence, it is unclear how to prepare a generalized Gaussian state.

Put differently, coherent and squeezed states of standard bosons always have a Gaussian Q function, and moreover zero stellar rank within the stellar-rank formalism introduced by [189, 190]. Conversely, a coherent or squeezed state of generalized bosons may not to have a Gaussian Q function, the clear classification of states in terms of their stellar rank will not be applicable in general case. In particular, the inner product between coherent states is not Gaussian see Eq. (A.18).

A.3.4 Gaussian Boson Sampling for Generalized Boson

Let us now derive the outcome probability of GBS for generalized boson and show that we still get a Hafnian by assuming our state has a Gaussian Q -function. To do so, we

write P_n as

$$P_n(\alpha) = \frac{1}{\prod_{i=1}^M f(n_i)^2} e^{\sum_{i=1}^M \ln(N(\alpha_i))} \prod_{j=1}^M \left(\frac{\partial^2}{\partial \alpha_j \partial \alpha_j^*} \right)^{n_j} \delta(\alpha_j) \delta(\alpha_j^*) \quad (\text{A.29})$$

We then evaluate the phase space integral (A.24) with the expressions for the Q function (A.28), and the P function (A.29), obtaining

$$\text{Pr}(\mathbf{n}) = \frac{1}{\prod_{i=1}^M f(n_i)^2} \frac{1}{g \sqrt{|\sigma_Q|}} \prod_{j=1}^M \left(\frac{\partial^2}{\partial \alpha_j \partial \alpha_j^*} \right)^{n_j} e^{\ln(N(\alpha) - \frac{1}{2} \alpha^\dagger \sigma_Q^{-1} \alpha)} \Big|_{\alpha_j \rightarrow 0}. \quad (\text{A.30})$$

From this, we recover standard GBS [6, 7] by choosing $N(\alpha) = e^{|\alpha|^2}$ and $f(n) = \sqrt{n!}$ because the expression in the argument of the exponential can be written as a quadratic form in the matrix $I_{2M} - \sigma_Q^{-1}$, where I_{2M} is the $2M$ -dimensional identity matrix.

Indeed, from the perspective of generalized bosons, it looks like for the standard boson case, the resulting expression is a miracle since we get the exponential quadratic term $e^{|\alpha|^2}$ for the normalization coefficient $N(\alpha)$. However, observe that only the second derivative on each mode contributes to the outcome probability if we only measure outcomes $n_j \in \{0, 1\}$ in every mode. This is because when letting $\alpha_j \rightarrow 0$ the exponential term will approach unity since $N(0) = 1$ for arbitrary generalized bosons. This corresponds to the second-order term in the series expansion of $\ln(N(\alpha))$ around $\alpha = 0$. Let us therefore compute the series expansion of $N(\alpha)$ in $|\alpha| = \sqrt{\alpha^* \alpha}$ around $|\alpha| = 0$ as

$$\ln(N(|\alpha|)) = c_0 + c_1 |\alpha|^2 + c_2 |\alpha|^4 + c_3 |\alpha|^6 + \dots \quad (\text{A.31})$$

As argued above, when restricting to $n_j \in \{0, 1\}$ for $1 \leq j \leq M$, only the term

linear in $|\alpha|^2 = \alpha^* \alpha$ will give a nontrivial contribution to the outcome probability. Hence, only c_1 is effective in this case, because all the higher order terms in $|\alpha|$ will be eliminated by $\alpha \rightarrow 0$. We obtain

$$\Pr(\mathbf{n}) = \frac{1}{\prod_{i=1}^M f(n_i)^2} \frac{e^{c_0 M}}{g \sqrt{|\sigma_Q|}} \prod_{j=1}^M \left(\frac{\partial^2}{\partial \alpha_j \partial \alpha_j^*} \right)^{n_j} e^{c_1 |\alpha|^2 - \frac{1}{2} \alpha^\dagger \sigma_Q^{-1} \alpha} \Big|_{\alpha_j \rightarrow 0}. \quad (\text{A.32})$$

Then we do the similar calculations as shown in Refs. [6, 7] which is based on the derivative expansion formula [191] converting partial derivatives of an exponential quadratic function to a summation over all perfect matching permutations (PMP) of product of matrix elements. Such a summation over PMP of products of matrix elements is exactly the Hafnian function. We have our final result:

$$\Pr(\mathbf{n}) = \frac{e^{c_0 M}}{g \prod_{i=1}^M f(n_i)^2} \frac{1}{\sqrt{|\sigma_Q|}} \text{Haf}(A_s) \quad (\text{A.33})$$

Here

$$A_s = \begin{pmatrix} 0 & \bigoplus_{i=1}^M c_1^{(i)} I_M \\ \bigoplus_{i=1}^M c_1^{(i)} I_m & 0 \end{pmatrix} (I_{2M} - \sigma_Q^{-1}). \quad (\text{A.34})$$

We finished the proof.

We also find that parallel results hold for the case of nonzero displacement. In this case, the Q function looks like:

$$Q_\rho(\alpha) = \frac{1}{g \sqrt{|\sigma_Q|}} e^{-\frac{1}{2} (\alpha - d_\nu)^\dagger \sigma_Q^{-1} (\alpha - d_\nu)}. \quad (\text{A.35})$$

We calculate the probability to observe a Fock state $|n_1, \dots, n_M\rangle$ where $n_i \in \{0, 1\}$ is

[191]. We arrive at

$$\Pr(\mathbf{n}) = \frac{e^{c_0 M} \exp \left[-\frac{1}{2} d_\nu^\dagger \sigma_Q^{-1} d_\nu \right]}{g \prod_{i=1}^M f(n_i)^2 \sqrt{|\sigma_Q|}} \prod_{j=1}^M \left(\frac{\partial^2}{\partial \alpha_j \partial \alpha_j^*} \right)^{n_j} \exp \left[\frac{1}{2} \boldsymbol{\alpha}^t A \boldsymbol{\alpha} + F \boldsymbol{\alpha} \right] \Big|_{\boldsymbol{\alpha}=0}. \quad (\text{A.36})$$

We get:

$$\begin{aligned} \Pr(\mathbf{n}) &= \frac{e^{c_0 M} e^{-\frac{1}{2} d_\nu^\dagger \sigma_Q^{-1} d_\nu}}{g \prod_{i=1}^M f(n_i)^2 \sqrt{|\sigma_Q|}} \sum_{\substack{j=1 \\ \pi_j \in \{2M\}}}^{|\pi|} \left[\left(\prod_{\substack{k=1 \\ B_j^1 \in \pi_j}}^{|B_j^1|} F_k \right) \text{Haf}(A_{B_j^2}) \right] \\ &= \frac{e^{c_0 M} e^{-\frac{1}{2} d_\nu^\dagger \sigma_Q^{-1} d_\nu}}{g \prod_{i=1}^M f(n_i)^2 \sqrt{|\sigma_Q|}} \left[\text{Haf}(A_S) + \sum_{j_1, j_2, j_1 \neq j_2} F_{j_1} F_{j_2} \text{Haf}(A_{S-\{j_1, j_2\}}) + \dots + \prod_j^{2M} F_j \right] \end{aligned} \quad (\text{A.37})$$

where the first sum is over all partitions of the set of $2M$ indices, the product is over all indices in the blocks B_j^1 and the remaining indices in blocks B_j^2 form $A_{B_j^2}$, a submatrix of A , which we then take the hafnian of.

A.4 Trapped-ion Implementation

In this section we discuss the details of physical implementation of the boson sampling protocol in trapped-ion setups.

A.4.1 Setup

The setup we have in mind is shown in Fig. 1 of the main text. More precisely we consider a chain of ions in a Paul trap. Each ion is considered to be a two-level system $\{|g\rangle_i, |e\rangle_i\}$ with the corresponding transition frequency ω_{eg} . We encode superspin $S^{(\alpha)}$ as collective excitation of a subset of ions $\{i\}_\alpha$ such that the lowering operator can be

defined as:

$$S_{\pm}^{(\alpha)} \equiv \frac{1}{\sqrt{N}} \sum_{\{i\}_{\alpha}} \sigma_{\pm}^{(i)}, \quad (\text{A.38})$$

where N is the number of ions encoding the superspin and $\sigma_{-}^{(i)} \equiv |g\rangle_i \langle e|$, $\sigma_{+}^{(i)} \equiv |e\rangle_i \langle g|$.

Mølmer-Sorensen interaction

As extensively discussed in the Ref. [89], the Ising-type interaction between of ions can be generated using the Moelmer-Sorensen [1] laser configuration. More precisely we consider a pair of bichromatic laser beams driving the transition $e \leftrightarrow g$ with the laser frequencies respectively tuned to $\omega_{eg} + \Delta$ and $\omega_{eg} - \Delta$ where Δ is some detuning having two different Rabi frequencies $\Omega_{\pm}$. Here we assume the possibility of selective driving of a pair of ions as shown in Fig. 1. This generates the ion-ion interaction characterized by the Ising Hamiltonian:

$$H_I = J_{i,j} \sigma_x^{(i)} \sigma_x^{(j)} + h \left(\sigma_z^{(i)} + \sigma_z^{(j)} \right), \quad (\text{A.39})$$

where the interaction coefficient scales as $J_{ij} = J_0 / |i - j|^{\zeta}$ with $0 < \zeta < 3$ and h denotes the transverse field.

A.4.2 Mode-mixing operation

In this section, we discuss the implementation of the two-mode mixing operation on a pair of superspins. More precisely we show how an interaction with the Hamiltonian $H_{\text{int}} = J^{(\alpha,\beta)} S_+^{(\alpha)} S_-^{(\beta)} + \text{H.c.}$ can be achieved in the setup described above. As discussed and experimentally demonstrated in [89] the basic XY Hamiltonian between any two spins can be achieved from the Ising Hamiltonian Eq. (A.39) in the limit of a large transverse field. In this case only the excitation-number preserving terms remain relevant and we find:

$$H_{i,j}^{(XY)} = J_{i,j} \left\{ \sigma_+^{(i)} \sigma_-^{(j)} + \text{H.c.} \right\} + h \left(\sigma_z^{(i)} + \sigma_z^{(j)} \right). \quad (\text{A.40})$$

Since the interaction preserves the number of excitations we can absorb the transverse-field term by transforming into the interaction picture with respect to it. The desired Hamiltonian H_{int} can be obtained in a Trotterized way by running the interaction Eq. (A.40) for each pair of ions for a time $\delta t_{i,j}$ inverse proportional to the interaction strength $J_{i,j}$ to preserve the spin symmetry Eq. (A.38) $\delta t_{i,j}^{\alpha,\beta} \approx \delta t_{\alpha\beta} \times \tilde{J}/J_{i,j}$, where $\tilde{J} = \min_{\{i\}_\alpha \{j\}_\beta} [J_{i,j}]$. To the lowest-order in Floquet-Magnus expansion we find:

$$\begin{aligned}
H_{\text{eff}} &\approx \frac{\sum_{i,j} \delta t_{i,j} J_{i,j} \left\{ \sigma_+^{(i)} \sigma_-^{(j)} + \text{H.c.} \right\}}{\sum_{i,j} \delta t_{i,j}} \\
&\approx J_0 N \frac{\sum_{\alpha,\beta} \delta t_{\alpha\beta} \times \left\{ S_+^{(\alpha)} S_-^{(\beta)} + \text{H.c.} \right\}}{\sum_{\alpha,\beta} \sum_{i,j} \delta t_{\alpha\beta} \times |i-j|^\zeta}
\end{aligned}$$

This Hamiltonian is equivalent to the Hamiltonian of interest H_{int} . We can now estimate the order of magnitude of the interaction strength for the nearest-neighbor superspins. Using [89, 192] $\zeta \approx 1$ and $J_0 = 1\text{kHz}$ we find the overall interaction constant for the nearest and next-nearest neighbor superspins being respectively $J^{(\alpha,\alpha+1)} \approx 44\text{Hz}$ and $J^{(\alpha,\alpha+2)} \approx 21\text{Hz}$. For comparison the typical decoherence rates can be estimated to be of the order of 1Hz [89].

A.5 Circuit-QED implementation

In this section we provide details of the circuit-QED implementation of the boson-pair generalized boson. The preparation step is discussed in the main text. Here we only focus on the implementation of the mode-mixing unitary operation. In this derivation we closely follow [72].

A.5.1 Mode-mixing Hamiltonian

We now consider the implementation of the mode-mixing unitary operation. Here for simplicity we only consider two cavities ($\omega_{i=1,2}$ denote frequency and a_i is the mode annihilation operator) which interact with four Josephson junctions (ω_J denote frequency

and J is the mode annihilation operator) and two two-level systems. The Hamiltonian of the system reads [72] $H = H_0 + H_d$:

$$H_0 = \omega_c \sum_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} + \omega_J \sum_{\lambda} J_{\lambda}^{\dagger} J_{\lambda} + \omega_0 c^{\dagger} c - \frac{E_J}{24} \sum_i \phi_i^4, \quad (\text{A.41})$$

$$H_d = \sum_i \Omega_i(t) J_i^{\dagger} + \text{H.c.}, \quad (\text{A.42})$$

where the phases are:

$$\phi_1 = \phi_a a_1 + \phi_b b + \phi_J J_1 + \text{H.c.},$$

$$\phi_2 = \phi_a a_2 + \phi_b b + \phi_J J_2 + \text{H.c.},$$

and $\phi_{a,b,J}$ denote the corresponding participation ratios. The Rabi frequencies are assumed to be given by:

$$\Omega_i(t) = \Omega_i e^{-i\omega_d t}$$

We now transform into the interaction frame with respect to the driving frequency ω_d and discard the rapidly rotating terms. Renormalizing the frequencies such as to include the Stark shifts due to driving the effective Hamiltonian can be put under the following form (we ignore quartic terms for b as we assume it does not contain more than 1 photon at the time):

$$H_{\text{eff}} = \sum_i \left(g_i a_i^{\dagger 2} c + \text{H.c.} \right) - \Delta c^{\dagger} c - \chi \sum_i a_i^{\dagger} a_i^{\dagger} a_i a_i,$$

where $g_i = -\frac{1}{2}\phi_b\phi_c^2\phi_J\frac{\Omega_i}{\Delta_J}$ is a complex effective tunneling coefficient, $\Delta_J = \omega_d - \omega_J$, and the induced quartic non-linearity is $\chi = \frac{\phi_c^4}{4}$. The detuning is denoted as $\Delta = 2\omega_a - \omega_0 - \omega_d$. In the following we will drop the on-site nonlinear term proportional to χ . As discussed in [72] it can be dynamically compensated by coupling to an additional Josephson qubit.

A.5.1.1 Adiabatic elimination of cavity bus

We now perform the adiabatic elimination of the cavity bus degree of freedom c assuming the driving is weak enough such that $g_i \ll \Delta$. The resulting Hamiltonian is

$$H_{\text{eff}} = \sum_{i,j} \frac{g_i g_j^*}{\Delta} a_i^{\dagger 2} a_j^2.$$

Now assuming the coupling coefficients are time-dependent $g_i = g_i(t)$ we can implement any coupling between any pair of sites in a Trotterized fashion in complete analogy to Sec. A.4.2.

A.5.2 Fock-state preparation

We now consider the preparation of Fock state $\frac{1}{\sqrt{2}}a_i^2|0\rangle$ in the system described by the Hamiltonian (A.41, A.42) but with the driving Hamiltonian to be of the form

$$H_d = \Omega_{\text{dr}} \sum_i \cos(\omega_{\text{dr}} t) (a_i + a_i^\dagger).$$

In rotating-wave approximation we get for each site:

$$H_{\text{eff}} = \frac{\Omega_{\text{dr}}}{2} (a_i + a_i^\dagger) - \Delta_a a_i^\dagger a_i - \chi a_i^\dagger a_i^\dagger a_i a_i$$

with $\Delta_a = \omega_{\text{dr}} - \omega_a$. We now assume the system is initially prepares in the Fock $|0\rangle$ state and the frequency of the drive is tuned into resonance with the two-photon resonance such that $\Delta_a = -\chi$. The system undergoes Rabi oscillations $|0\rangle \rightarrow |2\rangle$ with the Rabi frequency given by $\Omega_2 = \sqrt{2}\Omega_{\text{dr}}^2/(4\chi)$. The estimate of fidelity can be obtained by comparing the Rabi frequency and the corresponding detunings as discussed in the main text.

Appendix B:

B.1 Two-dimensional conformal field theories

In this section, we summarize the important aspects of the two-dimensional CFTs relevant to the results presented in this paper. Detailed discussions of two-dimensional CFTs can be found in Refs. [39, 40, 193].

The Virasoro minimal models are the complete set of unitary CFTs with a finite number of irreducible representations under the Virasoro algebra; however, if a CFT is also invariant under a larger symmetry group, it may be an RCFT by having a finite number of irreducible representations under the extended symmetry algebra. This is the case for parafermionic models and superconformal minimal models, which contain conserved parafermionic and fermionic currents respectively.

The two-dimensional CFTs we consider may be specified by a central charge, c , and a finite set of holomorphic and anti-holomorphic fields, denoted by $\phi_{h_L}(z)$ and $\phi_{h_R}(\bar{z})$ respectively. Here, we use complex coordinates $z = x + it$ and $\bar{z} = x - it$ to parametrize the two-dimensional coordinates (x, t) . The numbers (h_L, h_R) , which are called the conformal dimensions of the associated primary fields, are real numbers which are generically independent. With this data, it is known that the finite-size energy spectrum of a two-dimensional CFT (in units of $2\pi/L$) is given by Eq. (1), where the

lowest states correspond to primary fields, and the higher states are known as descendants. However, the degeneracy of the states corresponding to primary operators and their descendants can be nontrivial [194].

We now review the degeneracy structure of the energy spectrum. In this work, we simply present the result for the partition function and refer the reader to Ref. [39] for details. We consider an RCFT on a torus with complex-valued periods equal to ω_1, ω_2 , and define the modular parameter of the torus as $\tau = \omega_2/\omega_1$. Then we can write the partition function of an RCFT on the torus as [39]

$$Z(\tau) = \sum_{h_L, h_R} M_{h_L, h_R} \chi_{h_L}(\tau) \chi_{h_R}(\bar{\tau}), \quad (\text{B.1})$$

where

$$\chi_{h_{L,R}}(\tau) = \sum_{n=0}^{\infty} \dim(h_{L,R} + n) q^{h_{L,R} + n - c/24} \quad (\text{B.2})$$

are the so-called characters associated with a given primary operator $\phi_{h_{L,R}}$. Here, M_{h_L, h_R} counts the number of occurrences of the primary $\phi_{h_L}(z) \times \phi_{h_R}(\bar{z})$ in the CFT, and we use the parametrization $q = e^{2\pi i \tau}$.

The reason for considering the partition function on the torus is to demand that $Z(\tau)$ be left invariant under the modular transformations $\tau \rightarrow \tau + 1$ and $\tau \rightarrow -1/\tau$. This strongly constrains the structure of the spectrum investigated in the main body of the paper. It is believed that only modular invariant CFTs can be realized by a one-dimensional quantum lattice model, although non-modular invariant CFTs may arise as boundaries of two-dimensional lattice theories with bulk topological order [195]. In the

following we discuss the form of χ_{h_L} for the CFT families we are interested in.

B.1.1 Virasoro minimal models

In Virasoro minimal models, the central charge of the Virasoro algebra takes values of the type [106],

$$c_{p,q} = 1 - 6 \frac{(p-q)^2}{pq}, \quad (\text{B.3})$$

where p, q are coprime integers such that $p, q \geq 2$. Then the allowed conformal dimensions of the (anti)holomorphic representations are

$$h_{r,s} = \frac{(pr - qs)^2 - (p - q)^2}{4pq}, \quad \text{with } r, s \in \mathbb{N}^* \quad (\text{B.4})$$

where

$$1 \leq r \leq q - 1, \quad 1 \leq s \leq p - 1. \quad (\text{B.5})$$

The (p, q) and (q, p) models are the same.

From the previous discussion, we know that the allowed values of (h_L, h_R) and their degeneracies can be inferred by the set of modular invariant partition functions on the torus. The complete set of such partition functions has been entirely worked out for the unitary minimal models using the so-called ADE classification [196].

As a definite example, we consider the Ising CFT ($c = 1/2$), in which case there is only a single modular invariant choice of operators. If one expands the partition function in terms of the parameters $q = e^{2\pi i\tau}$, $\bar{q} = e^{-2\pi i\bar{\tau}}$, the full energy spectrum and its degeneracy can be read off from the coefficients and powers of the expansion. For the

Ising CFT, the partition function turns out to be diagonal, meaning one only allows fields of the form $\phi_{h_L}(z) \times \phi_{h_R}(\bar{z})$ with $h_L = h_R$, and we can read off the spectrum from the degeneracy of q alone. Just giving the q -dependence, and keeping terms up to q^5 and the level-3 descendants, the expansion is

$$q^{\frac{1}{12}(1-\frac{6}{3(4)})} Z_{ising} = 1 + \sqrt[8]{q} + q + 2q^{9/8} + 4q^2 + 3q^{17/8} + 5q^3 + O(q^{25/8}).$$

This expression should be read as follows: with energies measured with respect to the ground state and in units of $2\pi/L$, we have unique states with $E = 0, 1/8, 1$, a two-fold degenerate state with $E = 9/8$, a four-fold degenerate state with $E = 2$, a three-fold degenerate state with $E = 17/8$, etc. This explains how the energy level structure of the Ising model given in the main text was obtained.

B.1.2 $\mathbb{Z}_k$ parafermion CFTs

$\mathbb{Z}_k$ parafermion CFTs have a central charge given by $c = \frac{2(k-1)}{k+2}$ [106]. The conformal dimensions of the primary fields of these CFTs are

$$h_{r,s} = \frac{r(r+2)}{4(k+2)} - \frac{s^2}{4k}, \quad (\text{B.6})$$

where $r = 0, 1, \dots, k$ and $s = -r + 2, -l + 4, \dots, r$. The associated character is [197]

$$\chi_{(r,s)}(\tau) = \eta(q) c_s^r(q), \quad (\text{B.7})$$

where $c_s^r(q)$ is given by

$$c_s^r(q) = \sum_{l,m=0}^{\infty} (-1)^{l+m} q^{(k+r)lm + \frac{1}{2}(l+1)l + \frac{1}{2}(m+1)m} \times \\ \frac{q^{-\frac{c-1}{24} + h_{r,s}}}{\eta(q)^3} \left(q^{\frac{1}{2}l(r+s) + \frac{1}{2}m(r-s)} - \right. \\ \left. q^{\frac{1}{2}l(2k-r-s+2) + \frac{1}{2}m(2k-r+s+2) + k-r+1} \right),$$

and $\eta(q)$ is the Dedekind eta function. The partition function is then given by

$$Z(\tau) = \sum_{s=0}^{2k-1} \sum_{r=0}^k |\chi_{r,s}(\tau)|^2. \quad (\text{B.8})$$

One may show that the theories for $k = 1, 2, 3$ correspond to Virasoro minimal models, but for $k \geq 4$ we have new RCFTs. In this paper, we include parafermionic theories with $k = 4, 5, 6, 7$. The energy spectra of these models can be obtained by the q expansion of Eq. (B.8).

B.1.3 $\mathcal{N} = 1$ superconformal minimal models

The $\mathcal{N} = 1$ superconformal minimal models have central charge $c = \frac{3}{2} - \frac{12}{k(k+2)}$, with $k \geq 2$ an integer [106]. The scaling dimension of the primary field is

$$h_{r,s} = \frac{[(k+2)r - ks]^2 - 4}{8k(k+2)} + \frac{1}{32} (1 - (-1)^{r+s}). \quad (\text{B.9})$$

where $1 \leq r \leq k - 1$ and $1 \leq s \leq k + 1$. Fields with $r + s$ even have a conformal dimensions are given by:

$$h'_{r,s} = h_{r,s} + \frac{1}{2} + \delta_{r+s,2}. \quad (\text{B.10})$$

The characters and partition function for this case are much more involved, and we refer the readers to Refs. [198, 199] for their explicit expressions.

B.2 Details of the neural network architectures and training

In this section we present the details of the neural networks used in this work and explain the training process.

B.2.1 Supervised learning with energy spectra

For the supervised learning approach that led to results shown in Figs. 2 and 3 in the main text, we use the following neural network architecture with the input and output being the first 15 energy levels and their corresponding CFT class labels from the 13 CFT classes in Table 1 in the main text

$$\mathbb{R}^{15} \xrightarrow{\text{linear}} \mathbb{R}^5 \xrightarrow{\text{relu}} \mathbb{R}^{13} \xrightarrow{\text{softmax}} \mathbb{R}^{13} \quad (\text{B.11})$$

The layers are represented by their domain and the expressions above the arrows indicate the activation functions of each layer. To train the network we take samples of the energy spectra of different CFT classes and add a noise term drawn randomly from the uniform distribution in $(-\epsilon, \epsilon)$. This is physically motivated by the existence of

experimental measurement errors or subleading corrections to Eq. (3.1). It also serves as a form of data augmentation that can prevent overfitting [104]. We also preprocess the input such that the ground state energy is set to zero and the other energies are rescaled so that largest energy level is 1. This removes the contributions of the non-universal constants in the input data. We then optimize the categorical cross entropy over 3000 samples for each class with $\epsilon = 0.1$. The optimization is performed using the Adam optimizer with hyperparameters given in Ref. [200] in 2000 epochs with the batch size set to 128.

B.2.2 Supervised learning with Rényi entropies

For the results shown in Fig. 4 in the main text we use the following network architecture:

$$\mathbb{R}^n \xrightarrow{\text{relu}} \mathbb{R}^{100} \xrightarrow{\text{relu}} \mathbb{R}^{20} \xrightarrow{\text{relu}} \mathbb{R}^{15} \xrightarrow{\text{relu}} \mathbb{R}^{13} \xrightarrow{\text{softmax}} \mathbb{R}^{13} \quad (\text{B.12})$$

where n is the number of Rényi entropies we use. Similar to the classification of the energy spectra, we train the network by optimizing the cross-entropy using the Adam optimizer [200], this time with 500 epochs and batch size set to 128.

B.2.3 Unsupervised learning

We use the following architecture for the autoencoder used to obtain results shown in Fig. 5:

$$\mathbb{R}^{100} \xrightarrow{\text{relu}} \mathbb{R}^5 \xrightarrow{\text{sigmoid}} \mathbb{R}^h \xrightarrow{\text{relu}} \mathbb{R}^5 \xrightarrow{\text{sigmoid}} \mathbb{R}^{100}, \quad (\text{B.13})$$

where h is the dimension of the hidden variable ω . We train the network by optimizing C , using the Adam optimizer with 2000 epochs and batch sizes equals to 256.

B.3 Preprocessing procedure

In this section, we discuss how to eliminate the non universal constants E_0, E_1, L, v . We refer to this procedure as preprocessing. We have the following relation,

$$E = E_1 L + E_0 + \frac{2\pi v}{L} \left(-\frac{c}{12} + h_L + h_R \right). \quad (\text{B.14})$$

Let H_i be the i -th value of $h_L + h_R$, which is an integer. Notice that the lowest level, H_0 , is zero for all CFTs investigated in this work. Defining $\{X_0, X_1, \dots, X_n\}$ as our non universal energies, we have

$$X_i = E_1 L + E_0 + \frac{2\pi v}{L} \left(-\frac{c}{12} + H_i \right). \quad (\text{B.15})$$

We then have the energy differences from the ground state,

$$\frac{2\pi v}{L} H_i = X_i - (E_1 L + E_0) + \frac{2\pi v}{L} \frac{c}{12}. \quad (\text{B.16})$$

We then rescale the highest shifted energy to be 1. This gives a set of n preprocessed energies, $\{x_0, x_1, \dots, x_n\}$, given by

$$x_i = \frac{X_i - (E_1 L + E_0) + \frac{2\pi v}{L} \frac{c}{12}}{\frac{2\pi v}{L} H_n} = \frac{H_i}{H_n}. \quad (\text{B.17})$$

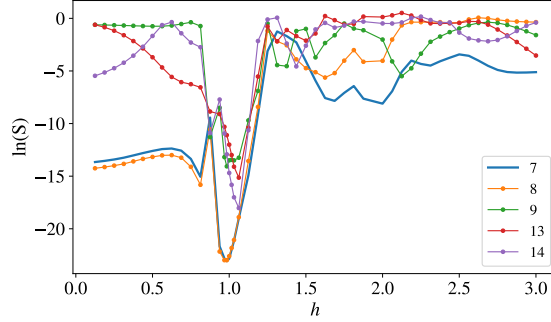


Figure B.1: We use a similar neural network model as in Fig. 2(a) in the main text, but train with different number of classes. The peak at $h = 1$ is stable in different models.

We see that x_i is independent of E_0, E_1, L, v .

B.4 Comparison of models trained using different classes

We train our neural network (same architectures) using the same spectral data, but change the number of classes in the training set. The rest of the parameters are kept the same as those used in Fig. 2(a) in the main text. In Fig. B.1, we observe that the critical point ($h = 1$) is visible in all cases and is stable. The less significant peaks, however, are not stable.

B.5 Comparison with the conventional method

Here we review two conventional methods (entropy scaling with system size and rescaled energy comparison) of extracting central charge from simulation or experimental data. These methods can be used separately or in combination with each other.

The first scheme relies on using the entropy scaling of the ground state. Specifically, it has been shown that the entanglement entropy S of a subsystem of size ℓ in the ground

state at one-dimensional $(1 + 1D)$ conformal critical points, is an extensive quantity that scales universally as [105, 201, 202]

$$S(L) = \frac{c}{3} \ln\left(\frac{L}{\pi a} \sin \frac{\pi \ell}{L}\right) + C_{A'} \quad (\text{B.18})$$

where c is the central charge, L is the length of the spin chain, a is the lattice constant, and $C_{A'}$ is a non-universal constant. Therefore, by finding the ground state, e.g., using numerical methods, and examining S at different values of L , for a subsystem size at a fixed relative length ℓ/L , one can obtain the central charge c from the slope of the linear-log plot of S versus L as shown in Fig. B.2a. After extracting the central charge we can find the corresponding CFT class by visually comparing the given energy spectrum with the CFT prediction in Eq. (B.14). We describe this approach in more detail in the following.

To visually compare the spectral data with CFT prediction, one needs to first rescale the data. We follow Ref. [106] and rescale energies such that the energy of first excitation in the CFT matches that of the data. As an example, in Fig. B.2b, we compare the spectral data of $H_T = 2H_1(1) + \lambda H_3$, where $H_1(h) = -\sum_{i=1}^L \sigma_i^z \sigma_{i+1}^z - h \sum_{i=1}^L \sigma_i^x$ and $H_3 = \sum_j \sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^z + \sigma_j^z \sigma_{j+1}^z \sigma_{j+2}^x$ at $\lambda \approx 0.856$, shown in gray lines with various CFT classes shown in color dots. As shown in the main text, this model is described by the minimal model (A_4, A_3) (CFT class 1 in Fig. B.2). Moreover, the central charge scaling can correctly identify this model as there is no other CFT with $c = 7/10$ in the CFT classes we considered. However, we observe that in the absence of the central charge value, it is not straightforward to find the correct CFT by visually inspecting Fig. B.2b. In contrast,

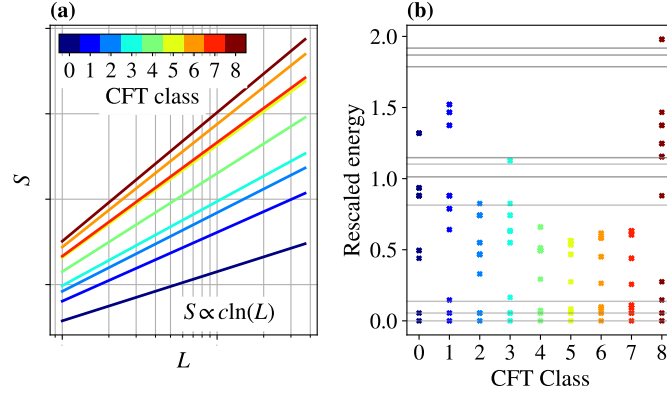


Figure B.2: (a) Scaling of the entanglement entropy S in the ground state at a conformal critical point as a function of the system size L . The slope of the linear-log plot gives the central charge c . (b) Visual comparison of the rescaled energies of a simulated model with predicted CFT energies. The correct CFT is class 1 corresponding to the (A_4, A_3) minimal model.

we use a different rescaling method, and by using the machine learning approach, we can quantify the similarity of the data to different CFT classes and identify the correct one (as shown in Figs. 2 and 3 in the main text) using the energy spectrum at a fixed system size.

Publications list in chronological order

1. **En-Jui Kuo** Yi Yang. "Extremal RN/CFT in both hands revisited." *Physics Letters B*, 2016 - Elsevier.
2. Heng-Yu Chen, **En-Jui Kuo**, H Kyono. "Anatomy of geodesic Witten diagrams" *Journal of High Energy Physics* 2017 (5), 1-40.
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