ENTANGLEMENT AND COMPLEXITY IN QUANTUM ELEMENTARY CELLULAR AUTOMATA

by Logan E. Hillberry © Copyright by Logan E. Hillberry, 2016

All Rights Reserved

A thesis submitted to the Faculty and the Board of Trustees of the Colorado School of Mines in partial fulfillment of the requirements for the degree of Master of Science (Applied Physics).

Golden, Colorado

Date _____

Signed: ______Logan E. Hillberry

Signed: _____

Lincoln D. Carr Thesis Advisor

Golden, Colorado

Date _____

Signed: _____

Jeff Squier Professor and Head Department of Physics

ABSTRACT

Complexity is an intuitively recognized feature of nature, but where does it come from? Is complexity only apparent at the classical level, or can it be found at the underlying quantum level as well? We approach these questions by exploring models consistent with basic quantum theory but which also hold promise for exhibiting complex behaviors – a set of models we call the quantum elementary cellular automata (QECA). Previously, various quantum cellular automata models have been studied for both their quantum information theoretic properties and their ability to simulate key physics equations like the Schrödinger and Dirac equations. We take the unique approach of analyzing QECA as complexitygenerating systems. Doing so requires a more precise notion of what we mean by complex. This is done by proposing nine axes of complexity along which the complexity of any system may be quantified. When applied to QECA, we find evidence of complexity using three of these axes, namely diversity, persistent dynamical macrostates, and connectivity.

The studies presented are numerical simulations done without approximation using highly optimized exact diagonalization code which supports a Hilbert space of up to 2²⁷ dimensions. The code is written entirely in the high-level open source programming language Python, making it easily expandable to future projects requiring exact simulation of quantum systems. A careful description of an algorithm critical to our method as well as our use of high performance computing resources on a cluster supercomputer is given.

Powerful quantifiers of entanglement and connectivity such as von Neumann entropy and complex network measures computed on quantum mutual information adjacency matrices provide analysis tools for the simulations. Each network measure is defined then tested on well-characterized entangled states from quantum information theory, like the GHZ and W states and singlet state arrays. The network measures known as network density, clustering coefficient, and disparity are specifically considered. We find these network measures offer unique information regarding the structure of two point correlations in the states produced by QECA dynamics, as compared to each other and as quantified by a principal component analysis.

Using such measures, we address the complexity of QECA models at three levels of specificity. First, a broad analysis of tens of thousands of simulations gives an overview of the variety of dynamics available to the models. We quantify the diversity of our simulations as the density of simulations which appear, on average, unlike typical entangled quantum states. Second, a more selective analysis identifies QECA by their complexity dynamics, in the frequency domain. A few QECA which exhibit persistent dynamical macrostates in the form of highly structured entanglement are also described. Entanglement dynamics are quantified by the distribution of changes in bond entropy (the von Neumann entropy of all bipartitionings of the QECA system). Finally, we take a detailed look at the transport properties, defined as the speed and diffusion rate of an initial localized excitation, in a QECA model found earlier to exhibit persistent dynamical macrostates. The transport properties are found to be a function of a model parameter called the phase gate angle. Additionally, for high phase gate angle we find the emergence of a second trajectory from a single initial excitation.

Taken together, the analyses in this thesis suggest QECA support elements of complexity in quantum dynamics. Since QECA are consistent with quantum theory, we conclude that complexity is not reserved for only the classical realm. The thesis finishes by suggesting future studies of complexity in quantum cellular automata.

TABLE OF CONTENTS

ABSTR	ACTiii
LIST OF	F FIGURES viii
LIST OF	F TABLESxi
LIST OF	F SYMBOLS xii
LIST OF	F ABBREVIATIONS xiv
ACKNO	WLEDGMENTS xv
DEDICA	ATION xix
CHAPT	ER 1 INTRODUCTION 1
CHAPT	ER 2 COMPLEXITY, QUANTUM MECHANICS, AND CELLULAR AUTOMATA
2.1	Complexity along nine axes
2.2	Complex network theory 12
2.3	Essentials of quantum mechanics 15
	2.3.1 The state vector and its dynamics
	2.3.2 The matrix representation and two-level systems
	2.3.3 Entanglement
	2.3.3.1 Entanglement by example
	2.3.3.2 Measuring correlation
2.4	Cellular automata
2.5	Quantum elementary cellular automata

CHAPT	FER 3 NUMERICAL TECHNIQUES FOR QUANTUM ELEMENTARY CELLULAR AUTOMATA SIMULATION	40
3.1	Requirements of simulations and useful computational tools	40
	3.1.1 Time evolution	41
	3.1.2 Measures	44
3.2	Algorithm for time evolution	44
3.3	High performance computing for quantum elementary cellular automata	48
CHAPT	ΓER 4 BROAD ANALYSIS	50
4.1	A mesoscopically large data set	50
4.2	Network measures for common entangled states	56
4.3	Equilibrium measure values	58
CHAPT	FER 5 COMPLEXITY DYNAMICS IN THE FREQUENCY DOMAIN	70
5.1	Discrete Fourier transforms	70
5.2	Spectral features of one-dimensional measures	72
5.3	Inspection of two-dimensional transforms	77
CHAPT	FER 6 THE APPROACH TO EQUILIBRIUM	82
6.1	Characterizing many body entanglement	82
6.2	Iteration-wise deviation	83
CHAPT	FER 7 SPEED AND DIFFUSION RATE	90
7.1	Center and diffusion of probability	90
7.2	Native and emergent transport	91
7.3	Transport properties and phase gate angle	93
CHAPT	TER 8 DISCUSSION AND OUTLOOK	. 100

8.1	Are quantum elementary cellular automata complex? 10)0
8.2	Suggestions for future work10)3
REFEI	RENCES CITED)6

LIST OF FIGURES

Figure 1.1	Schematic diagram of cellular automata update
Figure 1.2	Cellular automata as models of complexity
Figure 1.3	Examples of networks with different structure
Figure 2.1	Illustration of the Bloch sphere
Figure 2.2	Classical elementary cellular automata rules $R = 30, 90, \text{ and } 110. \dots 32$
Figure 2.3	Quantum circuit diagram of the QECA local transition operator
Figure 2.4	Circuit diagram for a single iteration of $MODE = SWP \dots 37$
Figure 2.5	Circuit diagrams for a single iteration of (a) MODE = ALT and (b) MODE = BLK
Figure 3.1	Memory consumption of the state vector for increasing system size
Figure 3.2	Time scaling of algorithm for efficient local operator application
Figure 4.1	Visualizing QECA dynamics with expectation values
Figure 4.2	Visualizing QECA dynamics with von Neumann entropy
Figure 4.3	Network measures of well-characterized entangled states
Figure 4.4	Network measures of well-characterized entangled and random states 60
Figure 4.5	Pincipal component analysis for Fock state initial conditions
Figure 4.6	Principal component analysis for entangled state initial conditions 61
Figure 4.7	Broad structure of QECA highlighting <i>L</i> dependence: Fock initial conditions
Figure 4.8	Broad structure of QECA highlighting S dependence: Fock initial conditions

Figure 4.9	Diversity of QECA broad structure: Fock initial conditions	66
Figure 4.10	Broad structure of QECA highlighting L dependence: entangled initial conditions	67
Figure 4.11	Broad structure of QECA highlighting S dependence: entangled initial conditions	68
Figure 4.12	Diversity of QECA broad structure: entangled initial conditions	69
Figure 5.1	Spectral features of rule 14	74
Figure 5.2	Spectral features of rule 4	75
Figure 5.3	Spectral features of rule 6	76
Figure 5.4	Summary of significant spectral features	78
Figure 5.5	Two-dimensional power spectrum of rules 4, 6, and 14	80
Figure 5.6	Two-dimensional power spectrum of rule 1	81
Figure 6.1	Bond entropy illustrating the structure of many body entanglement in QECA.	84
Figure 6.2	Aggregate distribution of Δs^{bond} for 1000 iterations	85
Figure 6.3	Average distribution of Δs^{bond}	87
Figure 6.4	Examples of the late-time evolution of bond entropy for $\theta = 0^{\circ}$	88
Figure 6.5	Examples of the late-time evolution of bond entropy for $\theta = 90^{\circ}$	89
Figure 7.1	Native rightward and leftward transport in rule 6	92
Figure 7.2	Emergent rightward and leftward transport of rule 6 with MODE=SWP \dots 9	93
Figure 7.3	Emergent rightward and leftward transport of rule 6 with MODE=BLK	94
Figure 7.4	Emergent rightward and leftward transport of rule 6 with MODE=ALT 9	95
Figure 7.5	Two-mode Gaussian mixture model used for peak and width finding of two trajectories under ALT update mode	96

Figure 7.6	Example linear fits for the extraction of transport properties of rightward propagation	97
Figure 7.7	Example linear fits for the extraction of transport properties of leftward propagation.	98
Figure 7.8	Transport properties for rule 6	99

LIST OF TABLES

Table 2.1	Types of quantum states
Table 2.2	Update table for rule $R = 30$
Table 2.3	QECA update table for Rule $S = 6$
Table 3.1	QECA simulation parameters
Table 4.1	Pairing QECA rules by symmetry

LIST OF SYMBOLS

single site index j, k
set of indices labeling neighborhood of site j \mathcal{N}_j
set of indices labeling all sites \dots \mathcal{L}
iteration index t
jk^{th} element of mutual information adjacency matrix \mathcal{I}_{jk}
network density \mathcal{D}
clustering coefficient \mathcal{C}
disparity \mathcal{Y}
state vector of system $ \Psi\rangle$
density matrix of system ρ
$n^{\rm th}$ computational basis state $ n\rangle$
projector onto subspace spanned by $ n\rangle$ \hat{P}_n
Hilbert space of system \dots \mathcal{H}
arbitrary Hermitian operator \hat{A}
probability of measurement outcome a $p(a)$
expectation value
von Neuman entropy $s^{\mathbf{v}^{\mathrm{N}}}$
classical cellular automata state x_j^t
phase gate angle θ
quantum elementary cellular automata rule number S

cellular automata rule numberR
the $2m + n$ digit of binary expansion of S S_{mn}
local update unitary V
local update pattern MODE
QECA global transition unitary $U_S^{\text{MODE}}(V)$
system size (number of sites) L
length of simulation (number of iterations) T
Hadamard gate H
phase gate $P(\theta)$
identity operator 1
power spectrum \mathcal{F}
spacetime grid for proabability of measuring a 1 $P_1(j,t)$
first moment of probability distribution P_1
second moment of probability distribution P_1 $\Delta_{P_1}(t)$

LIST OF ABBREVIATIONS

Quantum Elementary Cellular Automata	QECA
alternating update mode	ALT
block update mode	BLK
sweep update mode	SWP

ACKNOWLEDGMENTS

This work has benefited greatly from numerous interactions with many individuals. Here I would like to acknowledge the most impactful of these individuals.

First, I would like to thank my advisor Prof. Lincoln Carr, with whom I began working senior year. Prof. Carr has a way of motivating the very best in his students. His dedication to top-quality research, high expectations, and strong criticisms are the qualities which have shaped me the most. Prof. Carr has made enumerable useful research suggestions for this project, often guided by his powerful physical intuition, which he always so willingly shares with his students. The research and critical thinking skills I developed under Prof. Carr's guidance will follow me for the rest of my career, and for that I am truly grateful.

In addition to Prof. Carr, the defense of this thesis was overseen by two other professors in the Mines Physics Department. I would like to thank Prof. Susanta Sarkar for chairing my thesis committee. Additionally, Prof. Sarkar suggested an analysis technique which has played a vital role in this project and is the study of Chapter 6. Prof. Sarkar was always willing to discuss research and offer advice for my future education and research goals. The second Committee member, Prof. Mark Coffey, has deeply impacted my thinking as a physicist through our private discussions and classroom interactions. I have had the pleasure of learning programming techniques and computational physics from Prof. Coffey in two separate courses. These computational skills along with his insights into quantum walk, quantum lattice gas, and quantum computation literature have been immensely helpful in the preparation of this work. Together, Profs. Carr, Sarkar, and Coffey formed an incredibly talented thesis committee whose criticisms, suggestions, and advice have measurably improved the quality of the present work.

In the Summer of 2015, Prof. Simone Montangero of the University of Ulm Physics Department joined the Carr group as a visiting researcher. Prof. Montangero inspired the study of complexity in quantum cellular automata, the subject of this thesis, with an earlier publication on a similar model system. In addition to this inspiration, Prof. Montangero suggested an algorithm for the fast application of local operators to a composite quantum state. Before Prof. Montangero's visit, I was able to simulate a system size of 14 qubits. With his suggestions and continued optimization, I was eventually able to simulate 27 qubits. This contribution alone has enabled the studies presented in this thesis; however, Prof Montangero's contributions did not stop there. I am also deeply grateful for his thorough and insightful comments on an early version of this document and his continued input into the direction of the research as a whole.

Also in the Summer of 2015, I entered into a collaboration with Patrick Rall, Nicole Yunger Halpern, and Dr. Ning Bao of the Institute for Quantum Information and Matter at the California Institute of Technology. Patrick was an undergraduate researcher advised by doctoral student Nicole and postdoctoral fellow Ning. This research project was strongly supported by the Caltech team through weekly Skype meetings which have continued for an entire year. Patrick contributed greatly to this research in numerous way. First, he enabled my simulation code on a web browser, which aided in the analysis of hundreds of simulations and helped build our intuition for the systems we studied. Patrick also regularly performed impactful analysis on the data we generated and demonstrated an incredible motivation for the project long after his Summer research obligations were over. Additionally, Nicole and Ning brought a critical sense of maturity to the project from which I learned a great deal. Nicole's impetus and organization ensured regular progress, and her periodic check-ins with me were critical to my mental health in the trying times of this research. Ning brought an outstanding physical intuition to this project. It was often I felt myself describing a result in one of our Skype meetings and feeling I had lost the group in my explanations. Ning would follow up with a pertinent question or insightful comment that helped our longdistance collaboration click. I cannot overstate my deep gratitude for the Caltech team, their dedication, and their contributions.

From within the Carr group, I benefited from numerous conversations with my fellow researchers. Firstly, I'd like to thank David Vargas with whom I have worked closely since my first day in the Carr group. David's mathematical insights and knowledge of complex network theory shaped my understanding of this project. Daniel Jaschke is a superb programmer from whom I learned a great deal about writing custom quantum simulations. Daniel guided my development of several numerical tools like partial trace, bond entropy, and Trotter evolution algorithms. Gavriil Shchedrin informed this project by continuously asking the grounding question, "Where is the physics?" Gavriil's analytical prowess and intimate knowledge of two and three level quantum systems provided me with an endless resource of interesting conversation and physical insight. I am also grateful to the rest of the Carr group whose weekly research updates during group meetings allowed me to see a different but related facet of research in quantum many-body physics.

Finally, I would like to thank my professors and peers who have helped to shape my physical picture, of which there are too many to provide an exhaustive list. I would specifically like to acknowledge Profs. Lusk and Wu for teaching me quantum mechanics at the undergraduate and graduate levels. My peers Everett Hildenbrandt, Alexandra Nilles, Eric Jones, and David Grisham instilled in me a certain set of ideals when it came to programming. They taught me to use open source tools, to run Arch Linux, a do-it-yourself style operating system, and to never sacrifice code quality and comments in haste. These peers are amongst the brightest I have had the pleasure of working with. Their passionate curiosity was infectious, and our late night white board sessions brought about some of the most enlightening moments in my study. These memories are the fondest of my physics career thus far and I will carry them with me into my next chapter.

I am so fortunate to have been able to work on such open-ended and creatively demanding masters research. It was the support of the individuals mentioned here to which I owe my success. Furthermore, I owe thanks to the National Science Foundation for financial support during the Summer of 2015, and to my parents Jeff and Vicki Hillberry, my Grandmother Joyce Gust, and my Grandparents Darwin and Ruth Hillberry for their emotional and financial support.

To my parents, for their unwavering support and encouragement to follow my interests wherever they may lead.

CHAPTER 1 INTRODUCTION

This chapter introduces what we mean by complexity and makes a case for the importance of its study. Our discussion will naturally lead us to the question motivating this thesis: Does quantum mechanics give rise to the complexity we see around us?

In this thesis, the term *complexity* characterizes a system of multiple individuals which may interact in many ways resulting in collective group behaviors. We are not concerned with the many other uses of the word such as computational complexity, which studies the computational resources required to solve a problem and classifies the problem accordingly [1] or algorithmic or Kolmogorov complexity, the study of the shortest algorithm capable of generating some desired output [2]. Additionally, complexity is not chaos; chaos is related to the study of the sensitivity of a system to changes in initial condition. That being said, chaos is one mechanism for generating the complexity we are referring to [3]. Furthermore, complexity is not synonymous with complicated. In fact, we will soon discuss systems with simple descriptions which do exhibit complexity. Occasionally we will use "complex" to refer to a number of the form x + iy where x and y are real numbers and i is the imaginary unit $i \equiv \sqrt{-1}$, though context should make this case apparent. Finally, we note that complexity, as understood in this thesis, does not have a universally agreed upon definition, but rather the notion is typically conveyed with examples [4].

Let us return to what we do mean by complexity. Our characterization is intentionally general because the idea of a complex system is interdisciplinary. If the individuals are humans then the complex system in question could be the open-ended co-evolution of consumers and economic institutions [5], or the connectivity of social networks which are often structured in hierarchical or scale-free clusters [6]. Iron atoms in a dilute magnetic alloy are the individuals in a so-called spin glass. The interactions of the iron atoms give rise to an intricate state space responsible for anomalous dynamical behavior of spin glasses like irreversibility, aging, and memory effects [7]. Perhaps the field most concerned with complex systems is biology, since the interactions of species in an ecosystem, organs in an organism, cells in tissue, etc. are all by their nature complex according to our characterization. Thus, we have found examples of complexity across the disciplines of economics, sociology, physics, and biology.

Next, let us consider a certain hallmark of complexity, emergence, which describes when a system of individuals gives rise to group dynamics which are unpredictable even when given perfect knowledge of the individuals. What makes this feature so striking is that these emergent group behaviors are often rooted in simple, local rules followed by the individuals comprising the group. Take for example the behavior of a school of fish. No one fish is singled out as the leader, deciding where and how the school moves. Rather, each individual fish takes sensory input from its immediate fish neighbors (local information) then decides where and how to move in a way that maximizes conformity with the group (simple rules). The fish move in unison giving the impression of a single organism. That such emergence is observable in a variety of natural scenarios, from schools of fish, flocks of birds, and colonies of ants, to the fluid dynamics of a tsunami or Jupiter's Great Red Spot [8, 9], to the pattern of synapses in your brain allowing you to read these words, may be taken as evidence for the apparent preference of nature toward complexity.

A system exhibiting emergence is often considered complex. However, complex systems need not exhibit emergence. Instead, emergence is an element of a particular *axis of complex-ity*. We will give nine axes of complexity in Section 2.1 which are inspired by examples form various disciplines. In the meantime it suffices to note that emergent phenomenon are often expressed by a system as persistent dynamical macrostates, one of our axes of complexity. Further examples of our nine axes include diversity and connectivity. Diversity refers to the collection of unique individuals in a system, while connectivity describes the relations between individuals, both important aspects of our characterization of complexity. With

emergence, diversity, and connectivity in mind, we next consider complexity as it relates to physics.

The study of particles, their interactions, and their composition into extended bodies has always been the realm of physics. Progress in physics has long been made by carefully constructing approximations, simplifications, and reductions of physical situations while always being aware of the regimes of validity for these methods. Though immensely critical to our modern understanding of nature and our ability to devise new technologies, these methods leave a gap in our predictive power over systems which elude such simplifications, systems which may often be regarded as complex. For example, a system whose description is resistant to reductive analysis implies emergence; simplifications often limit the diversity of states in our physical system (e.g., thermodynamics is concerned with states in or near equilibrium); and assumptions of limited or nonexistent interactions are often explicitly made (e.g., in the kinetic theory of gases or short-range Ising models). Nonetheless, understanding complex systems in the context of physics is of technological and epistemological interest. To get a better picture for why reductive reasoning eventually fails, lets follow its recipe *ad absurdum*.

The atomistic view, first forwarded by Leucippus and Democrotis in 400 BC, posits that reality is reducible down to "atoms," which are indivisible units of reality, and the "void," the empty space serving as the arena for atoms [10]. This view has deeply impacted physical thinking, and its result, that there are irreducible elements of nature, has since been validated by modern particle physics. However, implicit in the atomistic view is the idea that reducibility is successful down to the scale of the indivisible atoms. That is, to completely understand a system, it is sufficient to completely understand the system's constituents. Taken to its extreme, the atomistic view would contend that a complete understanding of human social behavior is facilitated by a complete understanding of human individuals. Human individuals are understood through psychology and physiology, rooted in biology, in turn based on chemistry, which derives from atomic physics, built from the axioms of quantum mechanics. Thus, under the atomistic view, human social behaviors may be derived from the axioms of quantum mechanics, a statement hard to defend.

In our reduction of human social behaviors to the axioms of quantum mechanics, we passed through several branches of science. These transitions are not as smooth or well defined as suggested in the above. Instead scientists have given a unique name to a field when a new scientific framework offers a more efficient or more satisfactory explanation of natural phenomenon. The more efficient descriptions are often average theories which leave room for randomness, an important ingredient missing from the atomistic reduction of the complexities of human social behavior to the axioms of quantum mechanics. That being said, it is not at all clear that successive averaging procedures like, for example the transition from molecular dynamics to Hydrodynamics, will eventually result in e.g., human physiology. Moreover, quantum mechanics, our most successful and most fundamental physical theory, is inherently probabilistic. We are thus led to ask the question, at a fundamental level, does quantum mechanics give rise to the complexity we see around us?

While the question posed above is the motivation for the work presented in this thesis, answering it definitively is a tricky task that will likely take many researchers many more years to fully address. In any case, we will work toward answering this question using computational methods to simulate model quantum systems, quantify their dynamics, and assess their results as complex or not complex. Before outlining further details of our methods, we will describe the classical inspiration for our quantum models.

One way to study complex systems is to simulate them with computers, an approach we will rely on heavily in this thesis. A particular set of models that have been of considerable interest for some time are known as cellular automata [11, 12]. Cellular automata are discrete dynamical systems comprised of individuals which form a collective group. Each individual may always be found in one of a finite number of states. There are three important spatial scales in cellular automata. First and smallest is the scale of the individual, also called a site. Second there is the scale of a site's neighborhood, which is the set of sites which may

influence the next state of that site via local interactions. Finally there is the scale of the group, or the collection of all sites.

Cellular automata are also discretized in time. A transition of the group from one state to the next in time is called an iteration. A single iteration is complete after each site has had its state updated conditioned on the state of its neighborhood. The rule for updating a site based on its neighborhood is performed via a local transition function which encodes the resulting state for all possible neighborhood configurations. With a finite number of states available to sites and a finite sized neighborhood, there is a finite, though exponentially large, number of possible rules with which sites could be updated. The update process is outlined in Figure 1.1 and defined mathematically in Section 2.4. Cellular automata are useful models of complexity because one can control the size of the local state space and thus the potential for diversity among individuals. One can also control the size of the neighborhood and the precise form of the local interactions which govern cellular automata dynamics. Moreover, even the simplest of local update rules can give rise to surprising and often complex behaviors, like unpredictable long-time dynamics, fractal patterns, and computational completeness. In Figure 1.2 we compare the complexity of a living system to the pattern generated by a specific cellular automata rule.



Figure 1.1 Schematic diagram of cellular automata update. The state of each neighborhood (red, green, or blue) is supplied to the function f which encodes the cellular automata update rule and determines the next state of the center site in the neighborhood.



Figure 1.2 Cellular automata as models of complexity. (a) The shell pattern of *Conus textile*, a poisonous sea snail, is shown in panel. Interactions between individual cells secreting proteins and calcium carbonate give rise to the observed pattern. (b) The evolution of a centered local bit flip initial condition under a specific cellular automata rule is shown in panel. Time runs top to bottom and space left to right. Every cell transitions to a 0 (white) unless it is the center site in a neighborhood of the form 100, 011, 010, or 001 in which case the center site transitions to a 1 (black). Remarkably, this simple rule mimics the shell pattern in panel (a).

Seeking an answer our motivating question and inspired by the ability of cellular automata to capture our characterization of complexity, we implement a version of cellular automata consistent with quantum theory which we call the quantum elementary cellular automata (QECA). We will give a precise mathematical description of QECA in Section 2.5. Furthermore, our use of high performance computing facilities, outlined in section 3.3, allows us to rapidly simulate QECA for a variety of parameters. We develop metrics for understanding QECA dynamics and interpret the results through the lens of complex systems. In particular, some of our most quantitative results will come from analyzing the connectivity of correlations in QECA dynamics. We will be investigating connectivity with the mathematical framework of complex network theory. In this framework, individuals are represented as nodes and there interactions as links between nodes. Together, the links and nodes form a network, or graph, which illustrates the connectivity of the system. See Figure 1.3 for an examples of networks with various structure. Complex network measures may then be applied to graphs to quantify the structure of their connectivity. We will specifically consider the scalar-valued network measures known as network density, clustering coefficient, and disparity which quantify the density, transitivity, and uniformity of connections, respectively. We give mathematical definitions of these measures in Section 2.2.



Figure 1.3 Examples of networks with different structure. Nodes are black circles and links between nodes are gray lines. Complex network theory is concerned with classifying networks and the structure of their connections with complex network measures.

With our model and methods in place, a natural first question to ask is what types of quantum states are available to our QECA model? We approach this question in Chapter 4 by considering the long-time average of our measures for over ten thousand simulations, each with varied model parameters and initial states. This gives a broad, average view of the quantum states our QECA generate. Comparing these results to a few well characterized entangled states from quantum information theory illustrates the diversity of QECA dynamics.

Once we have better intuition for the broad structure available to our models, we take a closer look at the dynamics of a few QECA. This analysis reveals immense structure in dynamics which was hidden by the average picture taken in the broad analysis. In Chapter 5, discrete Fourier transforms are used to better understand the dynamical features of connectivity in QECA dynamics. Then, in Chapter 6, evidence for persistent dynamical macrostates is found for a few of our QECA models, though these dynamics are typically quite sensitive to a free parameter in our models. However, one rule is found with long-time behavior which remains dynamic and is uniquely robust to changes in model parameters, a rule we will come to know as rule S = 6. Our observation of the unique properties of rule S = 6 lead us to our most focused analysis which aims to quantify the transport properties of the rule. That is, when initiated simulations with a localized excitation, this rule transports the information of the initial excitation back and forth throughout the dynamics. We quantify the speed and diffusion of this transport and identify a second trajectory which emerges from the single initial excitation for certain model parameters.

From these three analyses operating at an increasingly focused scope, we conclude that elements of complex systems like persistent dynamical macrostates, emergence, diversity, and connectivity are present in some QECA. There is however a larger fraction of our models which appear non-complex, at least within the scope of the analyses presented here. We conclude this thesis with a discussion of the complex features observed in our QECA models and suggest future directions for the use of quantum cellular automata as models of complexity at the micro scale.

CHAPTER 2

COMPLEXITY, QUANTUM MECHANICS, AND CELLULAR AUTOMATA

In this chapter, we begin by taking a closer look at what we mean by complexity. We will also introduce the essentials of quantum mechanics required by this research. Then, after a brief introduction to the basics of cellular automata, we conclude the chapter with a construction of our QECA scheme. By the end of the chapter, we will have laid out all of the most critical theoretical tools used in this thesis.

2.1 Complexity along nine axes

In Chapter 1 we introduced the term complexity to characterize a system of multiple individuals which may interact in many ways resulting in collective group behaviors. There, we also met cellular automata as a set of models capable simulating this type of complexity with simple local rules. While we can create models which simulate complexity such as cellular automata, we lack a set of principles predicting it generally. In this way, complexity is a phenomenon driven study. Contrast this with the laws of thermodynamics which provide a predictive framework with which to describe many large scale systems. While limited in the variety of systems it describes (i.e., typically systems in or near equilibrium), thermodynamics has been exceedingly useful in building the technology of our modern world. As the basis of heat and energy transfer, thermodynamics has enabled technological milestones such as engines, generators, and refrigeration. Understanding how complex systems such as the internet, social relationships, ecologies, gene networks, and the brain arise as a consequence of physical law may allow us to predict and control complexity. With predictive power over the complex, our society could benefit from a technological revolution like the one incited by the formulation of thermodynamics in the beginning of the 19th century.

A first step towards a theory is to characterize quantitatively the object of study. As an initial attempt in this direction, we have developed *nine axes of complexity*. Each axis describes an aspect of complexity displayed by physical systems [13]. We do not claim these axes form a basis for complexity; the principal axes of complexity remain to be identified, though our nine axes do provide a starting point. The nine axes are as follows:

1. Multiscale hierarchies

Take for example the brain, where biologists have identified at least 7 different length scales important for cognition from neurotransmitters to axons [14]. Additional examples include the fractal patterns exhibited by certain bacteria colonies [15] or the intricate food webs of the rainforest, relating organisms from bacteria to insects, to top predators like jaguars.

2. Persistent dynamical macrostates

Living organisms, for example, are incredibly complex chemical systems persisting through time so long as they're alive. Another example mentioned in Chapter 1 is the great red spot on Jupiter or tsunamis on Earth. These are particular examples of emergent phenomenon, which may also appear in materials as rigidity, magnetism [16], quasi particles (i.e., Exciton-polaritons [17]), etc.

3. Non-Gaussian statistics

Specifically, we have in mind fat-tailed distributions, in which rare events are not so rare at all. Mathematically, this means complex systems often exhibit power law probability tails as opposed to the Gaussian or exponential tails seen in e.g. the distribution of student grades [18].

4. Fractional geometries

For example, many biological systems live somewhere between two and three dimensions, characterized by a fractional dimension [19]. Such systems are often fractallike, exhibiting bumpy, wrinkled, folded, or otherwise multiscale environments such as those in the brain, lungs, and intestines, or even the shorelines of Earth's land-water interfaces. Additionally, dissipative dynamical systems often follow fractal strange attractors [20] which provide good statistical predictability and characterize chaos.

5. Astronomically large probability spaces

In other words, complex systems often have available to them a large number of unique configurations, though the system often only explores a local region of them. The dynamics of protein folding can be seen as complex along this axis. Contrast this with a box of gas in thermal equilibrium with its environment in which, even if only a small number of possible configurations are realized during our observation time, a representative sample is explored [7].

6. Multiple constraints and trade-offs

For instance, robustness vs. fragility trade-offs in immunosenescence [21, 22] or volume constraints [23] which have clearly given rise to large surface areas in the form of wrinkly, bumpy surfaces in various organs of multicellular organisms and organelles of single cells. Other examples may come from model quantum systems with tunable interaction parameters. Phase transitions are typically found in these models when the strengths of certain competing interactions are comparable to one another [24], suggesting a link between criticality and complexity.

7. Diversity

Many complex systems have numerous distinct actors making up the cast. For example the human gut is a microbiome supporting hundreds or thousands of species [25]. Meanwhile there is only one variety of electron, with two spin states, in a crystal.

8. Selection principles

Natural selection is a mechanism of evolution which gives rise to the diversity of the life we find on earth. It is not clear if this aspect of complexity is unique to biological systems, but expanding our notion of selection principles to adaptivity more generally allows us to be more inclusive. We may then include systems like self-healing nanostructures [26], and even computational tools like genetic algorithms, and deep neural networks used in machine learning applications like speech recognition [27].

9. Connectivity

Complex systems often exhibit numerous interacting parts. Parts may be strongly, weakly, or not at all interacting with each other, defining an abstract network of connectivity. Representing objects by nodes and interactions between objects as edges on a graph gives us a way to quantify the structure of connectivity via *complex network measures*. Examples of connected complex systems include flight maps of the world's airports, the internet, food webs, metabolic pathways, etc. As a well developed quantitative tool currently available to the study of complex systems [28], we will repeatedly return to the idea of connectivity as quantified by complex networks. Thus, it is worth taking a closer look at the theory of complex networks.

2.2 Complex network theory

With the nine axes of complexity, we have refined our notion of complexity from the one sentence characterization given in Chapter 1. As we already mentioned, the axis of connectivity as quantified by complex networks will provide us with a set of quantitative tools for complexity. Here we give a very brief overview of the theory of complex networks relevant to this thesis.

We begin by supposing we are studying a system composed of parts which we may consider as the set nodes of a complex network. The relationship between parts may be described by a single, real, positive number, the edge strength. The collection of edges and nodes of a network may then be represented by an *adjacency matrix* \mathcal{A} . The value of the matrix element \mathcal{A}_{jk} gives the edge strength connecting node j to node k. If $\mathcal{A}_{jk} \in \{0, 1\}$, the network is said to be *unweighted*, otherwise, the network is *weighted*. Furthermore, for weighted networks, we will take the normalization $0 \leq \mathcal{A}_{jk} \leq 1$. If $\mathcal{A}_{jk} = \mathcal{A}_{kj}$ the network is said to be *undirected*, otherwise it is *directed*. Clearly undirected networks are represented by symmetric adjacency matrices. If $\mathcal{A}_{jj} = 0$, then the network does not permit self connections. In this thesis, we deal exclusively with weighted, undirected complex networks which do not permit self connection.

Once we have an adjacency matrix representing our complex network, there are several quantities which may be computed from it, known as complex network measures. These complex network measures are designed to quantify the structure of connectivity in the network. The measures also offer information compression because they are maps from matrices to scalars. The study of complex networks and their measures encompasses a broad and rich field, though we will focus on just three network measures. The interested reader is directed to [29] for more information.

The *network density*, denoted \mathcal{D} , is the average connection strength between nodes of a network. Let us consider an adjacency matrix for L nodes. Then, \mathcal{D} is given by,

$$\mathcal{D} = \frac{1}{L(L-1)} \sum_{j,k=0}^{L-1} \mathcal{A}_{jk}.$$
(2.1)

If \mathcal{D} is large (note $\mathcal{D} = 1$ maximally since we have $\mathcal{A}_{jj} = 0$), then each node is likely linked to many other nodes in the network, meaning the network is dense. Food webs are often dense networks [30].

Transitivity refers to the relationship between two bodies given that the same relationship holds between each body and a third intermediate body. Abstractly, a transitive relation between three bodies A, B, and C states $(A \sim B) + (B \sim C) \rightarrow A \sim C$. The zeroth law of thermodynamics is a transitive law, stating that if bodies A and B are in thermal equilibrium and bodies B and C are in thermal equilibrium then bodies A and C are also in thermal equilibrium. The *clustering coefficient*, C measures the degree of transitivity in a network and is given by

$$C = \frac{\text{Tr}(\mathcal{A}^3)}{\sum_{k \neq j}^{L-1} \sum_{j=0}^{L-1} ([\mathcal{A}^2]_{jk})}.$$
(2.2)

We can interpret C as the ratio of triangles to connected triples (triangles with one missing leg) in the network and thus a measure of transitivity. The larger the value of C, the more transitive, or clustered, the network is. Social networks are typically highly clustered because friend groups tend to be more common than isolated friendships [6].

Our last network measure is one which measures the uniformity of connections within the network. A nonuniform network is called disparate. The disparity of node j, denoted \mathcal{Y}_j , may be computed as

$$\mathcal{Y}_{j} = \frac{\sum_{k=0}^{L-1} (\mathcal{A}_{jk})^{2}}{\left(\sum_{k=0}^{L-1} \mathcal{A}_{jk}\right)^{2}}.$$
(2.3)

Then, the average disparity of the network is

$$\mathcal{Y} = \frac{1}{L} \sum_{j} \mathcal{Y}_{j}.$$
(2.4)

Though Eq. (2.4) is technically the average disparity, we will refer to it as simply the *disparity* because we will not be concerned with the node-wise disparity given in Eq. (2.3). Disparate networks typically display a strongly connected backbone linking several smaller, more weakly connected clusters of nodes. This measure is constructed such that

$$\mathcal{Y} = \frac{1}{L-1} \tag{2.5}$$

for a perfectly homogeneous network, given by

$$\mathcal{A}_{jk} = a, \quad \mathcal{A}_{jj} = 0. \tag{2.6}$$

where a is a real, positive constant. The homogeneous network has all nodes connected uniformly with strength a, except for self connection, and displays the minimum disparity. One example of a disparate network is that of a metabolic network. Metabolic networks show pathways of biomolecules through a variety of intricate processing channels. Many of these processing channels are secondary to the primary role of the biomolecule in the organism. Disparity has allowed researchers to filter metabolic networks to elucidate their primary function, effectively filtering out the secondary processes [31]. Our application of complex network theory will be to an adjacency matrix which comes from quantities arising in quantum mechanics. Armed with a clearer picture of complexity and specific quantitative tools from complex network theory, our next task is to recall the calculus of quantum mechanics required to develop QECA and the measures for characterizing their dynamics.

2.3 Essentials of quantum mechanics

Much of the classical world is best understood through the study of matter and light with the theories of Newton and Maxwell. In the early 1900's, Newton's theories of motion and Maxwell's theories of electromagnetism provided a sufficient understanding of our world save a few unanswered questions.

One of theses questions was explaining the spectrum of black body radiation. The black body spectrum refers to the distribution of frequencies (colors) emitted by a perfectly absorbing (black) material in thermal equilibrium with its environment. The solution to this theoretical problem was found by Max Planck in 1900 who quantized the energy of theoretical oscillators making up the radiating black body [32]. Planck's quantization procedure was a theoretical device employed in a "desperate act" to give a mathematical form to the black body spectrum [33].

Then, in 1905, Albert Einstein found a similar quantization useful in his analysis of the photoelectric effect [34]. Einstein found that electromagnetic energy is absorbed in discrete chunks which we now call photons. Einstein's theory explained existing experimental results but overturned the accepted undular (wave-like) theory of electromagnetic radiation $a \ la$ Maxwell.

Planck's explanation of the black body spectrum and Einstein's explanation of the photoelectric effect relied on exactly the same smallest unit, or *quanta*, of angular momentum, \hbar , known as the reduced Planck constant. By the 1920's, Planck's constant and the idea of quantization permeated the emerging theory of *quantum mechanics*. We've given a very brief history of the birth of quantum mechanics. Next we will briefly review import elements of the mathematical framework of quantum mechanics needed for our study of QECA.

2.3.1 The state vector and its dynamics

The mathematical formulation of quantum mechanics, at least the non-relativistic, manybody, closed system flavor we will be considering, is underpinned by a set of five postulates. These postulates describe how to represent a system; how to represent observables; how to measure observables of the system and how such measurement affects the system; how the system evolves through time; and how treat identical particles. We will now review the five postulates of quantum mechanics.

Postulate 1: In quantum mechanics, the system is described by a state vector. In Dirac notation, the state vector is written as a ket $|\Psi\rangle$. The state vector is a unit vector in a complex-valued, linear vector space with an inner product (a Hilbert space) denoted \mathcal{H} . This essentially means that state vectors can be scaled by complex numbers and added to one another and the result is always another state vector. Dual to every ket $|\Psi\rangle$ we have the bra $\langle\Psi|$, together forming a bra(c)ket $\langle\Psi|\Psi\rangle$, which denotes the inner product of $|\Psi\rangle$ with itself on the Hilbert space in which $|\Psi\rangle$ resides. Since $|\Psi\rangle$ is a unit vector its inner product must be unity: $\langle\Psi|\Psi\rangle = 1$.

The state vector is an abstract mathematical object which provides the probabilities associated with any measurement that can sensibly be made on the system. The inner product of the state vector with itself being unity expresses the sum of probabilities being one, as expected. Despite its name, $|\Psi\rangle$ is not a vector *per se*, but rather a ray because multiplication of $|\Psi\rangle$ by a phase factor $e^{i\phi}$ does not affect the probabilities of any measurement outcome for the system. For a more mathematically complete description of Hilbert spaces see [35].

Just as a vector in three dimensions may be expanded into a set of basis vectors $\mathbf{r} = x\hat{x} + y\hat{y} + z\hat{z}$, the state vector may be expanded into a set of basis state kets $\{|n\rangle\}$ as

$$|\Psi\rangle = \sum_{n} \langle n|\Psi\rangle |n\rangle.$$
(2.7)
The ability to perform this expansion implies our basis is *complete*,

$$\sum_{n} |n\rangle \langle n| = \sum_{n} P_{n} = \mathbb{1}$$
(2.8)

where we have introduced the projection onto the subspace spanned by the n^{th} basis state vector $P_n = |n\rangle \langle n|$ and $\mathbb{1}$ which denotes the identity operator on our system's Hilbert space.

Quantum theory also provides us a way to compound subsystems into an aggregate system. If our system is composed of L subsystems, the state vector of our system resides in the Hilbert space formed by the *tensor product* of the individual Hilbert spaces. Mathematically,

$$\mathcal{H} = \mathcal{H}_0 \otimes \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{L-1} = \bigotimes_{j=0}^{L-1} \mathcal{H}_j.$$
(2.9)

If each subspace has dimension

$$d_j = \dim(\mathcal{H}_j) \tag{2.10}$$

and is spanned by the set of basis kets $\{|n_j\rangle\}$ with $n = 0 \dots d_j - 1$, then the Hilbert space of our composite system has dimension

$$D = \dim(\mathcal{H}) = \prod_{j=0}^{L-1} d_j \tag{2.11}$$

and is spanned by

$$\{|N\rangle\} = \bigotimes_{j=0}^{L-1} \{|n_j\rangle\}$$
(2.12)

In the theory of closed quantum systems, the state vector for a system of L subsystems may always be written

$$|\Psi\rangle = \sum_{N=0}^{D-1} \langle N|\Psi\rangle |N\rangle.$$
(2.13)

If the state vector may be written in the less general form

$$|\Psi\rangle = \bigotimes_{j=0}^{L-1} |\phi_j\rangle \tag{2.14}$$

with each $|\phi_j\rangle$ of the form given on Eq. (2.7) it is said to be *separable*, otherwise it is said to be *entangled*. In this way, entanglement refers to the ability of a system to be described the

state of its constituent subsystems.

Separable states have subsystems described by *pure* states while the subsystems of entangled states are necessarily *mixed*. Pure quantum states are perfectly well described by the state vector while mixed quantum states describe a classical mixture (or ensemble) of different pure quantum states, each with their own unique state vector. The mathematical representation of mixed states requires the notion of a *density operator*, also called a density matrix and denoted ρ , on \mathcal{H} . For pure states,

$$\rho = |\Psi\rangle \langle \Psi|, \qquad (2.15)$$

while for mixed states, we have

$$\rho = \sum_{i} r_{ij} \left| a_i \right\rangle \left\langle a_j \right| \tag{2.16}$$

for an arbitrary basis $\{|a_i\rangle\}$ which spans \mathcal{H} . By diagonalizing the matrix described by entries r_{ij} , we may write

$$\rho = \sum_{i} p_{i} |\Psi_{i}\rangle \langle \Psi_{i}| = \sum_{i} p_{i} \rho^{(i)}$$
(2.17)

where $\{|\Psi_i\rangle\}$ is the basis which caries out the diagonalization and p_i are interpreted as the probability of having the pure state $\rho^{(i)} = |\Psi_i\rangle \langle \Psi_i|$ in the mixture. Normalization requires

$$\operatorname{Tr}(\rho) = \sum_{i} p_{i} = 1.$$
(2.18)

Additionally, ρ is a positive operator, meaning its eigenvalues are positive and possibly zero. In closed-system quantum mechanics, the state of the system is always pure, but the state of subsystems may be mixed. Moreover, both pure and mixed states can be either entangled or separable.

It follows that entangled mixed states must be written

$$\rho = \sum_{i} p_i \rho^{(i)} \tag{2.19}$$

while separable mixed states may be written

$$\rho = \sum_{i} p_{i} \bigotimes_{j=0}^{L-1} \rho_{j}^{(i)}.$$
(2.20)

where $\rho_j^{(i)}$ denotes the density matrix of subsystem j for the i^{th} component of the mixture. Table 2.1 summarizes the mathematical descriptions of pure, mixed, separable and entangled quantum states.

Table 2.1 Types of quantum states. Broadly, all quantum states can be regarded either pure or mixed and separable or entangled. For closed-system quantum mechanics, the state of the entire system is always pure; subsystems may be described by pure or mixed states; and both pure and mixed states can be either separable or entangled.

	Separable	entangled
pure	$ \Psi\rangle = \bigotimes_{j=0}^{L-1} \sum_{n=0}^{d_j-1} \langle n_j \phi_j \rangle n_j \rangle$	$ \Psi\rangle = \sum_{N=0}^{D-1} \langle N \Psi\rangle \Psi\rangle$
mixed	$\rho = \sum_{i} p_i \bigotimes_{j=0}^{L-1} \rho_j^{(i)}$	$ \rho = \sum_{i} p_i \rho^{(i)} $

When we develop QECA, we will describe the state of the group by a state vector. The state of the group lives in the Hilbert space constructed from the tensor product Hilbert spaces for each site. The Hilbert space of each site is taken to be two-dimensional. Such two dimensional Hilbert spaces describe the simplest possible quantum systems, called two level systems, which we explore more deeply in Section 2.3.2.

Postulate 2: Every observable in classical physics has a corresponding linear, Hermitian operator in quantum mechanics. A Hermitian operator \hat{A} satisfies the eigenvalue problem $\hat{A} |a\rangle = a |a\rangle$ and thus has the spectral decomposition $\hat{A} = \sum_{a} a |a\rangle \langle a|$. That \hat{A} is Hermitian means that $\hat{A} = \hat{A}^{\dagger}$ (i.e., \hat{A} is its own adjoint); the eigenvalues a are real; and the set $\{|a\rangle\}$ corresponding to unique a may be constructed as an orthonormal basis which is complete, i.e., $\sum_{a} |a\rangle \langle a| = 1$, on the Hilbert space $\mathcal{H} = \text{span}(\{|a\rangle\})$. In QECA, we will use operators defined on individual sites to help visualize the dynamics.

Postulate 3: Each eigenvalue of \hat{A} is a possible measurement outcome for observable \hat{A} . The corresponding eigenvector becomes the state of the system after $|\Psi\rangle$ is measured to yield a. The probability of obtaining a measurement result of a is found by expanding $|\Psi\rangle$ into \hat{A} 's basis as

$$|\Psi\rangle = \mathbb{1} |\Psi\rangle = \sum_{a} |a\rangle \langle a|\Psi\rangle = \sum_{a} \langle a|\Psi\rangle |a\rangle.$$
(2.21)

The quantity $\langle a|\Psi\rangle$ is known as the *probability amplitude* of measuring *a* for a system in the state $|\Psi\rangle$. The probability of measuring *a*, denoted p(a), is the absolute value squared of the probability amplitude

$$p(a) = |\langle a | \Psi \rangle|^2. \tag{2.22}$$

As long as $|\Psi\rangle$ is normalized and the $\{|a\rangle\}$ are orthonormal, we have $\sum_{a} p(a) = 1$.

Suppose one prepares many systems in an identical state $|\Psi\rangle$. Note that this ensemble is still pure because all the $|\Psi\rangle$'s are identical. Then, if \hat{A} is measured for each copy of $|\Psi\rangle$, the *expectation value* of this set of measurements, denoted $\langle \hat{A} \rangle$, is given by

$$\langle \hat{A} \rangle = \langle \Psi | \, \hat{A} \, | \Psi \rangle = \operatorname{Tr}(\rho \hat{A}) = \sum_{a} | \, \langle a | \Psi \rangle \, |^{2}a = \sum_{a} p(a)a.$$
(2.23)

Furthermore, it is possible that we want to compute the expectation value of an operator acting on a subsystem of our system. For this, we need a way of constructing the *reduced density matrix* of our subsystem from the density matrix of our system. This is done by tracing over the part of the system outside the subsystem of interest. To be specific suppose we have a system composed of L subsystems, enumerated by the set $\mathcal{L} = \{0, 1, ..., L - 1\}$. Suppose further we are interested in the expectation value of an operator \hat{A} which acts only on the collection of subsystems $\mathcal{N} \subset \mathcal{L}$. We must pad \hat{A} with identities so that it is the proper dimension to act on the state vector $|\Psi\rangle$ as $\hat{A} \otimes \mathbb{1}_{\mathcal{L}\setminus\mathcal{N}}$ where $\mathbb{1}_{\mathcal{L}\setminus\mathcal{N}}$ denotes the identity operator on the Hilbert space of all subsystems except those in \mathcal{N} . Then, for the expectation value we have

$$\langle \hat{A} \rangle = \operatorname{Tr}(\rho \hat{A} \otimes \mathbb{1}_{\mathcal{L} \setminus \mathcal{N}}) \tag{2.24}$$

$$= \operatorname{Tr}(\operatorname{Tr}_{j \notin \mathcal{N}}(\rho)\hat{A}) \tag{2.25}$$

$$= \operatorname{Tr}(\rho_{\mathcal{N}}\hat{A}) \tag{2.26}$$

where we have used the partial trace to construct the reduced density matrix

$$\rho_{\mathcal{N}} = \operatorname{Tr}_{j \notin \mathcal{N}}(\rho). \tag{2.27}$$

Using the last equality in Eq. (2.26) to compute the expectation value of local observables provides an efficient method for numerical calculation. The efficiency comes from avoiding the need to pad the local operator with identities which can quickly consume several gigabytes of memory in a computer for even moderately sized systems.

Postulate 4: The evolution of the state vector through time is governed by a unitary operator

$$|\Psi(t + \Delta t)\rangle = \hat{U}(\Delta t) |\Psi(t)\rangle. \qquad (2.28)$$

That \hat{U} is unitary means

$$\hat{U}^{\dagger}\hat{U} = \hat{U}\hat{U}^{\dagger} = \mathbb{1}.$$
 (2.29)

More importantly, unitary \hat{U} necessarily preserves the normalization of $|\Psi\rangle$ through time, which based on Eqs. (2.21) and (2.22) implies that unitary evolution conserves probability. Unitary time evolution also gives time reversal dynamics via the relation

$$\hat{U}(-\Delta t) = \hat{U}^{\dagger}(\Delta t). \tag{2.30}$$

Insisting the time evolution operator satisfies the composition law

$$U(t_2)U(t_1) = U(t_1 + t_2)$$
(2.31)

allows us to write

$$U(t) = [U(t/N)]^{N}$$
(2.32)

With a few more lines, one can deduce the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$
 (2.33)

where \hat{H} , known as the *Hamiltonian*, is typically the total energy operator and \hbar is Planck's constant (see [36] for an illuminating discussion). From this point onward, we choose units such that $\hbar = 1$.

Much of the study of quantum mechanics is concerned finding the Hamiltonian for a specific physical system and solving Eq. (2.33) to illuminate the system's unitary time evolution. However, our work is concerned only with constructing \hat{U} which hold potential for exhibiting complex dynamics. Similar considerations are often made in the field of quantum computing where the focus is less on finding Hamiltonians and more on devising systems of unitary operations for the sake of performing computations more securely [37] or efficiently [38] than is classically possible. When constructing QECA from the classical notion of cellular automata, we must take care in ensuring the resulting dynamics conserve probability and are reversible. Otherwise, our time evolution will not be consistent with the fourth postulate of quantum mechanics.

Postulate 5: Finally, the fifth postulate concerns the treatment of identical particles. Let the state of an L particle system be given by $|n_0 \dots n_j \dots n_k \dots n_{L-1}\rangle$ where we are only concerned with the state of two subsystems in the states $|n_j\rangle$ and $|n_k\rangle$. Since the subsystems are identical, exchanging their roles in the system must not affect the joint probability of obtaining a value a upon measurement of an arbitrary operator \hat{A} at each subsystem. That is,

$$|\langle a \dots a | n_0 \dots n_j \dots n_k \dots n_{L-1} \rangle|^2 = |\langle a \dots a | n_0 \dots n_k \dots n_j \dots n_{L-1} \rangle|^2.$$
(2.34)

It follows that the state vector itself may only change by an arbitrary phase factor $\gamma = e^{i\phi}$ upon exchange two identical subsystems according to

$$|n_0 \dots n_j \dots n_k \dots n_{L-1}\rangle = \gamma |n_0 \dots n_k \dots n_j \dots n_{L-1}\rangle.$$
(2.35)

However, upon a second exchange of the same two subsystems, the state vector must be completely unchanged, requiring

$$\gamma^2 = 1, \tag{2.36}$$

which restricts γ to be either +1 or -1. Systems for which $\gamma = 1$ are completely symmetric, are called Bosonic, and obey Bose-Einstein statistics while systems for which $\gamma = -1$ are completely antisymmetric, are called Fermionic, and obey Fermi-Dirac statistics. Note that for Fermionic systems, if the two subsystems are in identical states $|n_j\rangle = |n_k\rangle$ then the only resolution to Eq. (2.35) with $\gamma = -1$ is the null state vector. This is the origin of the so called Pauli exclusion principle [39]. There is no such restriction for Bosonic systems, allowing subsystems to coalesce into the same quantum state. This is the origin of Bose-Einstein condensation, which is known to give rise to nonlinear and emergent phenomenon [40]. It turns out that the notions of Bosonic vs Fermionic particles actually depends on the spatial dimension of the system. In fact, two dimensional systems may exhibit particles which are neither Bosonic or Fermionic. In one dimensional systems Bosons and fermions are dual to each other via a technique called Bosonization. Since our QECA system will be constructed in one spatial dimension, the fifth postulate of quantum mechanics will not be critical to our discussion, but is included here for completeness.

The postulates of quantum mechanics provide us with the basic tools for performing calculations. The exact interpretation and even the number of postulates is an open question, though one which is largely philosophical because any change to the underlying postulates cannot alter the calculations which agree with experimental observation. In the following section, we will work with the postulates as stated here to introduce specific models and measures which we will need for our QECA analysis.

2.3.2 The matrix representation and two-level systems

With the postulates of quantum mechanics laid out, we turn next to an important representation of state vectors and operators known as the *matrix representation*. To make this discussion as simple and relevant as possible, consider the simplest possible quantum system: a single 2-level system. Let's use the *computational basis* $\{|0\rangle, |1\rangle\}$. We will often refer to a 2-level system as a *qubit* in analogy to the classical bits of 1's and 0's in digital computation, but with the added structure of quantum mechanics. The correspondence between bits and qubits will be explicitly made when devising QECA inspired by cellular automata.

In general, the state of a two level system may be written as a superposition of the basis states $|\Psi\rangle = a |0\rangle + b |1\rangle$ with a and b complex-valued scalars, as in Eq. (2.7). We can view a and b as components of a two dimensional vector in a complex linear vector space using the matrix representation with the basis

$$|0\rangle = \begin{pmatrix} 1\\0 \end{pmatrix}, \ |1\rangle = \begin{pmatrix} 0\\1 \end{pmatrix}.$$
(2.37)

Normalization requires $|a|^2 + |b|^2 = 1$ which, combined with the fact that a global phase can always be factored out of the state vector, allows us to formulate the state of the qubit as

$$|\Psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle.$$
(2.38)

The density matrix of a (pure) qubit may be written (with the help of a few trigonometric identities)

$$\rho = |\Psi\rangle \langle \Psi| = \frac{1}{2} \begin{pmatrix} 1 + \cos\theta & \cos\phi\sin\theta - i\sin\phi\sin\theta\\ \cos\phi\sin\theta + i\sin\phi\sin\theta & 1 - \cos\theta \end{pmatrix}.$$
 (2.39)

The density matrix of a mixed qubit may be written as a sum of terms of the form (2.39), each scaled by the probability for that pure state to be in the mixed ensemble. A maximally mixed qubit has equal probability for all basis states of the Hilbert space to be in the ensemble. In general, for a maximally mixed quantum state

$$\rho = \sum_{n=0}^{D-1} \frac{1}{D} |n\rangle \langle n| = \mathbb{1}/D.$$
(2.40)

For qubits, we can see that the density matrix can be expanded into the basis

$$\sigma^{0} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \sigma^{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma^{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma^{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(2.41)

as

$$\rho = \frac{1}{2}(\sigma_0 + \mathbf{r}_{\Psi} \cdot \sigma) \tag{2.42}$$

where we've introduced the Bloch vector

$$\mathbf{r}_{\Psi} = r\sin\theta\cos\phi\hat{x} + r\sin\theta\sin\phi\hat{y} + r\cos\theta\hat{z}$$
(2.43)

and the vector of Pauli matrices $\sigma = \sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z}$. The inequality $0 \leq r \leq 1$ holds for the Bloch vector and r = 0 for a maximally mixed qubit while r = 1 for a pure qubit. Thus, we can represent the state of a qubit as a point on a unit-ball using \mathbf{r}_{Ψ} . This useful geometric visualization of the state of a qubit is called the *Bloch sphere* and is shown in Figure 2.1. Unfortunately, there is not a clean geometric picture of the state of a several-qubit system without significant information loss.



Figure 2.1 Illustration of the Bloch sphere, a useful geometric visualization for the state of a qubit. The state of an arbitrary qubit is represented by the Bloch vector, pointing from the origin to some point on the unit ball.

Since the Pauli matrices are unitary (note they are also Hermitian) they may be used to evolve the state of a qubit according to the fourth postulate of quantum .mechanics. In addition to the Pauli operators, we will be interested in the *Hadamard* and *phase* operators, or gates, denoted H and P, respectively. We give the matrix representation of H and Pin Eq. (2.44). Note that P is a function of a continuous parameter θ known as the *phase* gate angle. The action of the Hadamard gate on an arbitrary Bloch vector is visualized as a rotation about the \hat{y} axis by 90° followed by a rotation about the \hat{x} axis by 180°. Similarly, the phase gate is a rotation about the \hat{z} axis by θ .

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix}, \quad P(\theta) = \begin{pmatrix} 1 & 0\\ 0 & e^{i\theta} \end{pmatrix}$$
(2.44)

There are many beautiful mathematical structures within the two level system for describing quantum rotations and dynamics. For more information on the two-level system or quantum mechanics as a whole, we refer the reader to one of a number of excellent textbooks on the subject [41, 42]. We turn next to examining entangled states in a system of qubits.

2.3.3 Entanglement

Quantum entanglement is arguably the quintessential feature of quantum mechanics separating it from classical mechanics. Entanglement is essentially the idea that two physically distinct (though perhaps identical in nature) subsystems may give rise to a state of the system which cannot be understood as the composition of two pure states for each subsystem. In this section, we will explore a few important entangled states and various ways of quantifying correlation in quantum states.

2.3.3.1 Entanglement by example

In the language of Section 2.3.1, lets take the example of L = 2 and $d_0 = d_1 = 2$, i.e. a system of two qubits. We expect the dimension of our system to be 4, so we will call our basis states $\{|N\rangle\}$ for N = 0, 1, 2, 3. We can construct the basis for our system as the tensor product of the bases of our single qubit subsystems as

$$\{|N\rangle\} = \{|0\rangle, |1\rangle\} \otimes \{|0\rangle, |1\rangle\} = \{|0\rangle, |1\rangle\}^{\otimes 2} = \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$$
(2.45)

where we've introduced the convenient short hand $|mn\rangle = |m\rangle \otimes |n\rangle$. In the matrix representation, the tensor product is implemented as the *Kronecker product*. The Kronecker product for two arbitrary qubits is written

$$|\phi_0\rangle \otimes |\phi_1\rangle = \begin{pmatrix} a_0\\b_0 \end{pmatrix} \otimes \begin{pmatrix} a_1\\b_1 \end{pmatrix} = \begin{pmatrix} a_0\begin{pmatrix}a_1\\b_1\\b_0\\a_1\\b_1 \end{pmatrix} = \begin{pmatrix} a_0a_1\\a_0b_1\\b_0a_1\\b_0b_1 \end{pmatrix}.$$
 (2.46)

Thus, the matrix representation of the basis of our 2-qubit system is written

$$|0\rangle = |00\rangle = \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix}, \ |1\rangle = |01\rangle = \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix}, \ |2\rangle = |10\rangle = \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}, \ |3\rangle = |11\rangle = \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}.$$
(2.47)

We know that the state of our two qubit system can always be expanded in the basis of Eq. (2.47) as $|\Psi\rangle = c_0 |0\rangle + c_1 |1\rangle + c_2 |1\rangle + c_3 |3\rangle$ where the c_i are the probability amplitudes associated with $|i\rangle$. We also know that if our system cannot be written in the form of Eq. (2.46), it is entangled. As an example of entanglement, consider the state

$$|\psi_{-}\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle).$$
 (2.48)

Clearly, we have $c_0 = 0$, $c_1 = \frac{1}{\sqrt{2}}$, $c_2 = \frac{1}{\sqrt{2}}$, $c_3 = 0$. However if $|\psi_-\rangle$ is to be separable, we must have $c_0 = a_0 a_1$, $c_1 = a_0 b_1$, $c_2 = b_0 a_1$, $c_3 = b_0 b_1$, and we quickly run into a contradiction while solving this system of equations. Since $|\psi_-\rangle$ is not separable, we have shown that it is entangled.

The state $|\psi_{-}\rangle$ is known as the *singlet state*. The singlet state naturally arises in the study of angular momentum addition of two spin-1/2 particles. There are three other 2qubit states exhibiting similar entanglement which, when taken together with the singlet state, form an orthonormal basis for the two-qubit system and are collectively known as the *Bell states*, given by

$$|\phi_{\pm}\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle \pm |11\rangle\right), \qquad (2.49)$$

$$|\psi_{\pm}\rangle = \frac{1}{\sqrt{2}} \left(|01\rangle \pm |10\rangle\right). \tag{2.50}$$

Upon calculating the reduced density matrix for either qubit in a system described by any one of the Bell states, one finds the subsystem to be maximally mixed. This feature is quite remarkable because, as a composite system, the Bell states are pure, meaning there is no uncertainty about the quantum state of the system. Meanwhile, the component subsystems are maximally mixed, meaning there is maximal uncertainty of the subsystem's quantum state.

Moving to a system of more than two qubits, we can define two other important entangled states. The Greenberger – Horne – Zeilinger (GHZ) state may be written

$$|GHZ\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle^{\otimes L} + |1\rangle^{\otimes L} \right), \qquad (2.51)$$

while the W state is

$$|W\rangle = \frac{1}{\sqrt{L}} (|10...0\rangle + |01...0\rangle + \dots + |00...1\rangle).$$
 (2.52)

Notice that tracing out any one subsystem leaves $|GHZ\rangle$ in a separable mixed state but leaves $|W\rangle$ in an entangled mixed state.

2.3.3.2 Measuring correlation

If one splits an arbitrary quantum system into two parts, A and B, one may re-express the quantum state via the *Schmidt decomposition*

$$|\Psi\rangle = \sum_{i} \lambda_i |i_A\rangle \otimes |i_B\rangle \tag{2.53}$$

where the $|i_A\rangle$ are unitarily connected to some fixed orthonormal basis for subsystem A, call it $\{|m\rangle\}$, as $|i_A\rangle = \hat{U} |m\rangle$. Similarly $|i_B\rangle = \hat{V}^{\dagger} |n\rangle$. The proof of the Schmidt decomposition relies on the fact that we can always express the quantum state as $|\Psi\rangle = \sum_{m,n} C_{mn} |m\rangle \otimes |n\rangle$ for some matrix of complex numbers C_{mn} with singular value decomposition $C_{mn} = U\Lambda V^{\dagger}$. By the singular value theorem, U and V are unitary and $\Lambda = \text{diag}(\lambda_0, \lambda_1, \dots, \lambda_{d-1})$ where $\lambda_i \geq 0$ and d is the smaller dimension of the two Hilbert spaces \mathcal{H}_A and \mathcal{H}_B , $d = \min(d_A, d_B)$. The number of non-zero λ_i is known as the *Schmidt rank* and is equal to 1 if and only if subsystems A and B are separable. This property makes λ_i a useful tool for quantifying the entanglement between two parts of a system.

One important measure of entanglement is the von Neumann entropy of a reduced density matrix ρ_A , denoted $s^{\text{vN}}(\rho_A)$. The von Neumann entropy of subsystem A takes the form

$$s^{\mathrm{vN}}(\rho_A) = -\mathrm{Tr}(\rho_A \log_2 \rho_A) = -\sum_i \alpha_i \log_2 \alpha_i, \qquad (2.54)$$

and we define $0 \log 0 = 0$. The second equality in Eq. (2.54) is obtained by representing ρ_A in the basis of its own eigenvectors so that the α_i are the eigenvalues of ρ_A . Phenomenologically, $S^{\text{vN}}(\rho_A)$ tells us how much information we stand to gain, measured in number of qubits, by measuring system A.

We state without proof a few important properties of the von Neumann entropy (see [42] for a more complete discussion)

- $s^{VN}(\rho_A)$ is nonzero if and only if subsystem A is entangled with subsystem B.
- In a *d*-dimensional Hilbert space the entropy is at most $\log_2 d$ and saturates this bound if and only if the system is in a maximally mixed state.
- $s^{\text{vN}}(\rho_A) = s^{\text{vN}}(\rho_B)$ whenever the AB composite system is in a pure state.

This work will also make use of the quantum mutual information between two distinct subsystems A and B

$$\mathcal{I}(\rho_{A:B}) = s^{\mathrm{vN}}(\rho_A) + s^{\mathrm{vN}}(\rho_B) - s^{\mathrm{vN}}(\rho_{AB})$$
(2.55)

where ρ_{AB} denotes the density matrix of the AB composite system. The mutual information between two subsystems is the information common to both subsystems. The first two terms combine the information content of systems A and B (double counting the shared information). The third term then subtracts off the information content of the AB joint system, leaving us with only the information common to A and B. We will be particularly interested in $\mathcal{I}(\rho_{j:k})$ where j and k are single qubits in a 1-D lattice of L qubits. In this case, $\mathcal{I}(\rho_{j:k})$ for $i, j = 0, \ldots, L - 1$ defines a symmetric $L \times L$ adjacency matrix upon which we can calculate the network measures defined in Section 2.2. Network measures of the mutual information adjacency matrix allow us to quantify the structure of two-point correlations exhibited by a quantum state. This is because mutual information is bounded from below by any two point correlator [43], defined as

$$g_{jk}^{(2)}(\mathcal{O},\mathcal{O}') = \langle \mathcal{O}_j \otimes \mathcal{O}'_k \rangle - \langle \mathcal{O}_j \rangle \langle \mathcal{O}'_k \rangle, \qquad (2.56)$$

where \mathcal{O}_j (\mathcal{O}'_k) is an arbitrary observable on subsystem j (k). We have $g_{jk}^{(2)}(\mathcal{O}, \mathcal{O}') = 0$ if and only if measurements of \mathcal{O} at subsystem j are uncorrelated with measurements of \mathcal{O}' at subsystem k.

While network measures calculated on mutual information adjacency matrices are a very new tool available to the study of quantum states, they have been shown to detect quantum phase transitions in various models of physical systems (see [44]). A primary goal of this thesis is to test the utility of these network measures in quantifying the complexity of dynamical quantum systems, in particular QECA. We therefore turn to a more thorough description of cellular automata in the following section.

2.4 Cellular automata

Cellular automata (plural for cellular automaton) are dynamical systems which evolve on a discrete spacetime lattice [45]. In cellular automata, global dynamics are controlled by a simple local transition function. Each spatial discretization of the lattice, called a *site*, may be found in one of a finite number of states. The next state of a site may be updated using only local information of the site's *neighborhood* and the local transition function. A single temporal discretization of a cellular automata, known as an *iteration*, is complete once each site's new state has been computed and all sites have been updated simultaneously.

For concreteness, consider a one dimensional lattice of L sites, enumerated by the set $\mathcal{L} = \{0, \ldots, L-1\}$. Denote the state of the j^{th} site at iteration t by x_j^t . Each site may be found in one of k possible local states $x_j^t \in Q$, where Q is the k-member local state space. Further suppose our cellular automata have a contiguous neighborhood of N sites (take N to be odd). This means each site j has a neighborhood defined by the set of sites

 $\mathcal{N}_j = \{j - (N-1)/2, \dots, j, \dots, j + (N-1)/2\}$. The state of the neighborhood at iteration $t, x_{\mathcal{N}_j}^t$, is the list of the states of each site in that neighborhood at iteration t. This means that the state space of a neighborhood is the N-fold product space of the local state space $Q_N = Q^{\otimes N}$, so $x_{\mathcal{N}_j}^t \in Q_N$. Similarly, the state of the entire lattice at iteration t is described as $x_{\mathcal{L}}^t \in Q_L$ where $Q_L = Q^{\otimes L}$. Then, the local transition function is a map $f : Q_N \to Q$. To complete an iteration, f is simultaneously applied to all the neighborhoods in the lattice as a global transition function which is a map $F : Q_L \to Q_L$. In particular, we compute the state of the lattice at iteration t + 1 as

$$x_{\mathcal{L}}^{t+1} = F(x_{\mathcal{L}}^{t}) = \bigotimes_{j=0}^{L-1} f(x_{\mathcal{N}_{j}}^{t}.)$$
(2.57)

An exercise in combinatorics reveals that there are k^{k^N} possibilities for the local transition function f. Restricting ourselves to homogeneous cellular automata implies there are the same number of global and local transition functions. This is because homogeneous cellular automata are those with the same local transition function defined for all sites at all iterations. It is conventional to enumerate the possible f with integers $R \in [0, k^{k^N} - 1]$ which we may use to define the map $f : Q_N \to Q$. To do this, expand R into k^N digits as a base-k number. Then, enumerate the digits of this expansion from least significant to most significant with integers $r \in [0, k^N - 1]$. Expand r into N digits of base-k. Interpret the expansion of r as the neighborhood state which results in site j transitioning to the state given by the rth bit of the R expansion.

For a concrete example, consider the case with k = 2 and N = 3 on a 1D lattice of L sites, the so called *elementary cellular automata*. There are $2^{2^3} = 256$ elementary cellular automata which have been studied extensively [45]. In Table 2.2 we show an update table defining f for rule R = 30. In Figure 2.2 we show the evolution of rules R = 30, 90, and 110 with a single bit flip in the center of the lattice as the initial condition.

Using Table 2.2 notice that under rule R = 30 a neighborhood state of 011 could have had as a predecessor 011 or 001. Such irreversibility is introduced when neighborhood states with the same left and right neighbors require different actions to achieve the state specified by R. In rule R = 30, the neighborhood state 011 requires an identity operation on the center site while the 001 requires a bit flip on the center site. We highlight this sort of irreversibility here because it will be important to avoid in any quantum mechanical version of elementary cellular automata. Otherwise, the quantum version will not be consistent with the fourth postulate of quantum mechanics. We now turn to the precise construction of our QECA scheme.

Table 2.2 Update table for rule R = 30, an irreversible elementary cellular automata. Notice that the bits in the second row of this table form the number 30 in binary. It is understood that the left and right neighbors are unchanged during the local update.

bit significance (base 2), $x_{\mathcal{N}_j}^t$	111	110	101	100	011	010	001	000
rule number (base 2), x_j^{t+1}	0	0	0	1	1	1	1	0



Figure 2.2 Classical elementary cellular automata rules R = 30, 90, and 110. (a) R = 30, capable of generating encryption-quality random numbers [46], (b) R = 90, exhibiting a fractal structure known as the Sierpinski triangle, and (c) R = 110, which is capable of universal computation [47]. Time runs top to bottom and space left to right.

2.5 Quantum elementary cellular automata

Seven years after Feynman's first mention of a primitive quantum cellular automata in 1981 [48], researchers developed and simulated a quantum cellular automata model with an approximately unitary quantum transition function. This is where the term "quantum cellular automata" first appeared [49]. Today, the 1988 model has more in common with quantum walks (see [50]) than quantum cellular automata. A more formal quantum cellular automata model was then developed by [51] and furthered by several other authors [52, 53, 54]. The difficulty with this model lies in the difficulty of determining if a quantum cellular automata is "well formed." Essentially a well formed quantum cellular automata is one which adheres to the postulates of quantum mechanics as presented in Section 2.3.1.

Much of the existing quantum cellular automata research has focused on either the theoretical computational capabilities of quantum cellular automata [55], [56], the equivalence of various quantum cellular automata models [57], [58], or the reconstruction of fundamental quantum physics, e.g. solving the Schrödinger or Dirac equations or simulating quantum lattice gas models [59]). Additionally, entanglement dynamics are discussed and a construction of irreversible quantum cellular automata within the framework of open quantum systems is provided in [60]. The entanglement dynamics are used there to measure the distribution of entangled states for the purposes of quantum computation. Notably, the study of complexity generation in a Hamiltonian-based quantum cellular automata was initiated in [61]. However, the work presented in this thesis considers a broader class of quantum cellular automata and considers different quantifiers of complexity.

There is an entirely separate body of literature in which the term quantum cellular automata refers to quantum dot cellular automata [62, 63, 64, 65]. Quantum dot cellular automata is a field concerned with the design and fabrication of quantum dot-based cellular automata of the sort considered in Section 2.4. Quantum dots are nanometer scale semiconducting particles often considered for their applications in solar cells and biological imaging [66].

The study presented in this thesis is unique in that our focus in on QECA as complexity generating systems. That focus informs our choice of measures and analysis tools, e.g. complex network theory applied to quantum mutual information adjacency matrices. Our QECA is a quantum extension of the elementary cellular automata, so we will rely heavily on the details provided in Sections 2.3.1 and 2.4 in the following construction of QECA.

To start, we define our system to be a 1D lattice of L qubits. The state of the lattice at iteration t is restricted to be pure and thus is denoted $|\Psi(t)\rangle$. Our first task is to define the local transition function for QECA, or equivalently, adapt the numbering scheme of cellular automata to our QECA model. The fourth postulate of quantum mechanics demands that the local transition function be realized as a unitary operator; the nearest-neighbor interactions of elementary cellular automata suggest this unitary spans three qubits. Since unitarity implies reversibility, we are unable to simulate any QECA which exhibit irreversibilities such as rule 30 discussed in Section 2.4.

The requirement of reversibility suggests our QECA rule numbering scheme ought to be based on what action we preform on the center site (rather than the next state of the center site) and that our numbering scheme need only consider the left and right neighbors of the neighborhood, excluding the center site itself. Thus our QECA rules effectively have N = 2 and k = 2 resulting in $2^{2^2} = 16$ possible unitary QECA rules. We use $S \in [0, 15]$ to enumerate these rules. A one in the binary expansion of S corresponds to the application of a single qubit operator (the bit flip operator σ^x emulates classical elementary cellular automata, but is denoted V in the general case) to the center site, while a zero in the binary expansion corresponds to an identity operation. Thus rule S = 0 is the identity operator. If the local transition operator is to be unitary, then so to must be the single qubit operator V. Table Table 2.3 gives an example of an update table for rule S = 6. In general, from the update table for rule S we can construct a corresponding three qubit transition operator denoted $U_S(V)$. Our construction of $U_S(V)$ relies on expanding S into four digits of binary as

$$S = s_{11}2^3 + s_{10}2^2 + s_{01}2^1 + s_{00}2^0$$
(2.58)

This way, all of the information in S is encoded in a 2×2 matrix with elements s_{mn} . Then we may give an explicit form of $U_S(V)$ as

$$U_S(V) = \sum_{m,n=0}^{1} |m\rangle \langle m| \otimes V^{mn} \otimes |n\rangle \langle n|, \qquad (2.59)$$

where

$$V^{mn} = s_{mn}V + (1 - s_{mn})\mathbb{1}.$$
(2.60)

It is informative to represent $U_S(V)$ as a quantum circuit diagram, which we do in Figure 2.3. Quantum circuits are a graphical representation of quantum operations on a register of qubits. Each qubit connects to a horizontal wire which is fed into various quantum gates and time is thought of as flowing left to right. We take the convention that the top-most qubit in a circuit diagram represents the left-most qubit on our lattice; likewise, the bottom-most qubit in the circuit diagram represents the right-most qubit of the lattice. A gate connected by a vertical wire to a circle on another qubit's timeline represents a control operation. The qubit feeding into the gate is called the target and the qubit connected vertically to the gate is called the control. Control operations apply gates to the target qubit only if the control qubit is in the proper state.

Table 2.3 QECA update table for Rule S = 6. The first row describes the state of a center site's neighbors. The second row indicates whether or not to apply V to the center site. Notice that the bits in the second row of this table construct the number 6 in binary.

j-1,j+1 angle	$ 11\rangle$	$ 10\rangle$	$ 01\rangle$	$ 00\rangle$
Apply Gate to center site? (s_{mn})	0	1	1	0

Now that we know how to define the local unitary transition operator for QECA, we need to address how to define an iteration. Recall Eq. (2.57) which defined an iteration for cellular automata as the simultaneous application of the local transition function to all sites of the lattice. The only way to preform this operation is by making a copy of the state so

$$\begin{array}{c} |q_{j-1}\rangle \\ |q_{j}\rangle \\ |q_{j+1}\rangle \end{array} = \begin{array}{c} \swarrow \\ - \bigg) \\ - \bigg)$$

Figure 2.3 Quantum circuit diagram of the QECA local transition operator. Filled circles represent control-on-1 operations, open circles represent control-on-0 operations, and x'd circles represent a linear combination of these two control operations.

that one copy may be read from while the other is written to. This way each read operation is unaffected by any other write operations.

However, the case for QECA is complicated by the *no cloning theorem* [67], which prohibits ever making a copy of a quantum state. Our solution is to relax the requirement of a simultaneous update for each iteration. This relaxation is equivalent to allowing for a specific order in which each site will be updated and thus allowing earlier local updates to influence later local updates. We then write a global update as,

$$|\Psi(t+1)\rangle = \prod_{j \in \text{MODE}} U_S(V) \otimes \mathbb{1}_{\mathcal{L} \setminus \mathcal{N}_j} |\Psi(t)\rangle$$
(2.61)

$$\equiv U_S^{\text{MODE}}(V) \left| \Psi(t) \right\rangle \tag{2.62}$$

where $\mathbb{1}_{\mathcal{L}\setminus\mathcal{N}_j}$ denotes the identity operator for all sites except for the neighborhood of site jand MODE is a set specifying the order in which sites are to be updated. For the purposes of this thesis, we consider three possible orderings. Our three modes are given the names sweep (SWP), alternate (ALT), and block (BLK). The SWP mode begins by updating site j = 0. The update is then swept across the lattice to site j = L - 1, so SWP = $\{0, 1, \ldots, L - 1\}$. The ALT mode first updates all the even-indexed sites then all odd-indexed sites. Since the application of $U_S(V)$ centered on site j may only alter site j, the update of all sites with an index of the same parity may occur simultaneously. Finally, the BLK mode updates all sites with index $j \mod 3 = 0$, then all sites with index $j \mod 3 = 1$, and finally all sites with index $j \mod 3 = 2$. The circuit diagram for the SWP mode is shown in Figure 2.4. The circuit diagrams for the ALT and BLK modes are shown in Figure 2.5.



Figure 2.4 Circuit diagram for a single iteration of MODE = SWP with L = 9. Information is maximally transferred rightward (downward in the circuit diagram) at rate of L sites per iteration. Leftward, (upward in the circuit diagram) information transfer is maximally one site per iteration.

Specifying the mode of our QECA defines the update procedure for all but the boundary qubits. The qubits at the boundaries may be updated once we specify the boundary conditions of our simulation. Periodic boundary conditions may be achieved by defining the neighborhoods $\mathcal{N}_0 = \{L - 1, 0, 1\}$ and $\mathcal{N}_{L-1} = \{L - 2, L - 1, 0\}$. For fixed boundaries, define the index labels j = l and j = r to always be referring to a site with a fixed state on the left or right end of the lattice, $|q_l\rangle$ and $|q_r\rangle$ respectively. We can then use Eq. (2.59) to define a two-site local update operator for the left and right boundary qubits as



Figure 2.5 Circuit diagrams for a single iteration of (a) MODE = ALT and (b) MODE = BLK with L = 9. Under MODE = ALT information can maximally travel at two site per iteration in either direction. Under MODE = BLK, information can maximally travel at three sites per iteration rightward (downward in the diagram) or two sites per iteration leftward (upward in the circuit diagram).

$$B_S^{(l)}(V) = \sum_{m,n=0}^{1} \langle m | q_l \rangle V^{ln} \otimes | n \rangle \langle n |$$
(2.63)

$$B_S^{(r)}(V) = \sum_{m,n=0}^1 |m\rangle \langle m| \otimes V^{mr} \langle n|q_r\rangle$$
(2.64)

All of our simulations will have boundaries fixed to $|q_l\rangle = |q_r\rangle = |0\rangle$.

We now have completely defined our family of QECA models. Each QECA requires a rule number S defining how neighbors influence a qubit's update, a unitary single qubit operator, V, with which we update each site conditioned on the state of its neighbors, and an update mode specifying the sequence in which individual qubits are to be updated. In this chapter we have also carefully described what we mean by complexity, reviewed the essentials of quantum mechanics, and given a mathematical treatment of cellular automata. The next chapter is devoted to implementing our QECA formalism numerically.

CHAPTER 3

NUMERICAL TECHNIQUES FOR QUANTUM ELEMENTARY CELLULAR AUTOMATA SIMULATION

In this chapter we will introduce a few of the key numerical techniques and considerations applicable to the simulation of QECA. All of the code for this project has been written in Python 3.5 and is freely available at [68]. We will begin by summarizing the features of QECA and the measures upon them which our simulations must consider. We will then describe an efficient algorithm for exact QECA time evolution. Finally, the high performance computing architectures used to simulate QECA are reviewed.

3.1 Requirements of simulations and useful computational tools

Broadly, the simulation of QECA requires two tasks, time evolution and measurement. Time evolution consists of representing the state in the computer and evolving it in time according to Eq. (2.62). By measurement, we mean applying all the measures of interest, e.g. Eqs. (2.54), (2.1), (2.2) and (2.4), to the state vector at each iteration. These tasks are described in detail in the next two section, but our focus now is on the Python libraries found to be useful in developing our QECA code base.

In addition to standard scientific computing libraries available for Python i.e., Numpy, Scipy, and Matplotlib, our code makes use of the *hdf5 file system* via the Python library h5py [69]. This system allows us to create one file with the .hdf5 extension into which we save the results of time evolution and the associated measures. Data can be saved to or accessed from the .hdf5 file at any point in the simulation. More importantly, data from the file may be accessed without loading the entire file into memory. Thus the hdf5 file system allows us to create a single data file for each simulation while still while still retaining the ability to load the results of a single measures at a time. Since this project is exploratory, we would like to be able to run many simulations as quickly as possible. To this end, we have implemented a batch parallelism scheme for running many independent simulations simultaneously. Because simulations are independent of one another, this parallelism can be achieved with just a few lines of code using the Python library mpi4py [70]. This implementation offers a huge time savings when on multicore processors. Most modern day personal computers have at least a few cores. Even more simulations can be ran in parallel when working with advanced high performance computing architectures with hundreds of cores. We will take a closer look at the use of high performance computing for simulating QECA in Section 3.3, but next we describe the computational tasks of time evolution and measurement.

3.1.1 Time evolution

Time evolution will be done without approximation. This means we will not be using matrix product state algorithms like the density matrix renormalization group method of time evolving block decimation [71, 72]. MPS algorithms are typically used to simulate large systems with low entanglement. Because of the high degree of entanglement present in many of our QECA, which is explored in Chapters 4 and 6, MPS algorithms fail to offer significant simulation advantages after just a few iterations. Because our simulations are exact, we will be dealing with the entire Hilbert space of our system; this space grows exponentially base 2 with each additional qubit. Thus, our simulations face no challenges simulating highly entangled dynamics, but struggle to simulate large systems.

To get a feel for the difficulty caused by an exponentially growing state space, consider the quantum state of L qubits. The quantum state is stored in the computer in the matrix representation using the computational basis as a vector of 2^L complex, double precision (64 bit) floating point numbers. Each complex number has a real and imaginary part so the number of bytes (recall there are 8 bits per byte) required to store a single state vector is

$$N_{\rm bytes} = 16 \times 2^L = 2^{L+4}.$$
(3.1)

From Eq.(3.1) we can see that L = 16 requires about 1.04 megabytes of memory while L = 26 requires about 1.07 gigabytes of memory to store $|\Psi\rangle$. We are able to run simulations with L = 27 sites which requires about 2.1 gigabytes per state vector to store in the computer. This theoretical scaling is explicitly tested in Figure 3.1.



Figure 3.1 Memory consumption of the state vector for increasing system size. The amount of memory required to store the matrix representation of the state vector of an L-qubit system is measured to increases exponentially with L. The theoretical prediction is given by Eq. (3.1). The exponential growth is base two, as expected, since the number of components in the matrix representation is equal to the dimension of the Hilbert space which increases exponentially in L with base two.

Since the size of the state vector grows so rapidly with L, we will only ever hold one state vector in memory at a time. In Python 3.5 this is implemented with the generator data type. Furthermore, we will not save the states we compute to the hard drive either. Instead, each time a state vector s computed in a simulation, we immediately calculate all the one and two site reduced density matrices and save those. This representation of the state offers significant compression over the full quantum state and still allows us to compute sitewise expectation values using Eq. (2.26) and the mutual information adjacency matrix using Eqs. (2.54) and (2.55). We also have the ability to compute and save the reduced density matrix describing any bi-partitioning of the lattice, though this can drastically increase both simulation time the size of output files.

To be fulley defined, QECA simulations need several parameters to be specified, most of which we have already met. In addition to the three parameters required to specify the update sequence (i.e., V, S, and MODE), we need to specify L, the length of the lattice and T, the number of iterations to simulate. We also must have some way of specifying the initial condition of the lattice. Specifying the initial condition is equivalent to specifying all 2^L complex numbers initially representing $|\Psi\rangle$. Since making this specification is very cumbersome, even for even moderately sized systems, we would like to have simple ways of specifying useful initial conditions. To do this, we have written a string parsing function which can create computational basis states and common entangled states like the GHZ, and W states, defined in Eqs. (2.51) and (2.52), given simple input strings. Table 3.1 collects all the simulation parameters and a short description of their purpose. Each parameter in Table 3.1 is in one-to-one correspondence with an input parameter in the main module of our QECA code base.

Table 3.1 QECA simulation parameters. Specifying these six parameters fully defines the QECA simulation. Using batch parallelism, our code can simultaneously perform many simulations with varied parameters. The exact number of simulation which can be performed simultaneously depends on the computer architecture running the code. We have performed up to 72 simulations simultaneously using a cluster-based super computer.

parameter	description
	Lattice length
T	No. iterations to simulate
S	QECA rule number
V	Single qubit unitary
MODE	Update ordering
initial condition	String describing initial state

3.1.2 Measures

For each simulation, we will also compute a suite of measures in addition to the reduced density matrices. For each iteration, these include all one and two site expectation values of the Pauli operators $\langle \sigma_j^{\alpha} \rangle$ and $g_{jk}^{(2)}(\sigma^{\alpha}, \sigma^{\alpha})$ for $j, k = 0, \ldots, L - 1$ and $\alpha = x, y, z$ as defined in Eq. (2.56). We also compute and save the site-wise von Neumann entropy, the quantum mutual information adjacency matrix \mathcal{I} , defined in Eqs. (2.54) and (2.55), and the three network measures \mathcal{D}, \mathcal{C} , and \mathcal{Y} computed on the adjacency matrix, defined in Eqs. (2.1), (2.2), and (2.4). Furthermore, the code is easily configured to also measure the bipartite von Neumann entropy and correlators of the form $g_{jk}^{(2)}(\sigma^{\alpha}, \sigma^{\beta})$ with $\alpha, \beta = x, y, x$, though such correlators are not considered in this thesis due to the fact that they bound from below the quantity of interest, namely quantum mutual information [43].

3.2 Algorithm for time evolution

The ability to exactly simulate 27 qubits in a high-level scripting language like Python took several optimization layers. Furthermore, the only way we are able to keep the simulations exact and reach this system size is because Eq. (2.62) is exactly local. Often local evolution schemes are used as an approximation for more general systems via the *Trotter* expansion [73]. We have found that our algorithm for QECA simulations works equally well for the Trotter expansion, although such simulations are approximate. In any case, it is very useful to have a function which accepts an *n*-site operator, a list of *n* site indices, and a state vector and returns a new state vector with that operator applied only to the provided indices. We'll call this function op_on_state.

One obvious way to simulate the time evolution of Eq. (2.62) is to explicitly construct $U_S^{\text{MODE}}(V)$ as the product of $L \ 2^L \times 2^L$ matrices. This procedure is very memory intensive and quickly saturates several gigabytes of random access memory for just L = 14. We will call this "big matrix method" version zero of the op_on_state function. As system size increases, the big matrix becomes more sparse, making sparse matrix methods an appealing option.

A sparse matrix is essentially a data structure which stores the row index, column index and value of every nonzero value in an array. Sparse arrays typically provide considerable memory savings and speed up when the array is less than 5% non-zero. However, we can do better than standard sparse array methods by leveraging out knowledge of the tensor product structure of the state vector. The method we develop here will be for a system of qubits for simplicity, however our code provides support for a list of sites with arbitrary local dimension.

Consider a three qubit system in a separable state. Let the state of the j^{th} qubit be given by $|\psi_j\rangle = a_j |0\rangle + b_j |1\rangle$. The full state vector is then given by

$$|\Psi\rangle = \begin{pmatrix} a_0 a_1 a_2 \\ a_0 a_1 b_2 \\ a_0 b_1 a_2 \\ a_0 b_1 b_2 \\ b_0 a_1 a_2 \\ b_0 a_1 b_2 \\ b_0 b_1 a_2 \\ b_0 b_1 a_2 \\ b_0 b_1 b_2 \end{pmatrix} = \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \\ c_7 \end{pmatrix}.$$
(3.2)

Next consider an operation on qubit j = 2 as $\hat{A} \otimes \mathbb{1}_{0,1} |\Psi\rangle$ where \hat{A} is some single-qubit operator. Notice that information about site j = 2 has entered into every component of the system's state vector. More generally, every component of the system's state vector depends on some component of the state of each subsystem. Thus, if we wish to update the state of $|\psi_2\rangle$ with \hat{A} , we potentially have to update every component of $|\Psi\rangle$. This updating can be done with only \hat{A} and $|\Psi\rangle$ without the need for padding \hat{A} with identities. To do this, regroup the components of $|\Psi\rangle$ into a list of 4 ordered pairs, each ordered pair contains one component with an a_2 factor and a second with a b_2 factor. The list of components in this case is given by $\{\{c_0, c_1\}, \{c_2, c_3\}, \{c_4, c_5\}, \{c_6, c_7\}\}$. Then operate \hat{A} on each of the pairs, and reshape the components back into the original order. If instead one wanted to operate on site j = 1, use the grouping $\{\{c_0, c_2\}, \{c_1, c_3\}, \{c_4, c_6\}, \{c_5, c_7\}\}$. Similarly, for site j = 0the appropriate grouping is $\{\{c_0, c_4\}, \{c_1, c_5\}, \{c_2, c_6\}, \{c_3, c_7\}\}$. The next generation of the op_on_state function, version one, used this idea to greatly increase the number of sites that could reasonably be simulated. However, version one needed to create a list of indices with which it selected the proper components of $|\Psi\rangle$ to be fed into \hat{A} . The third and final version of op_on_state, version two, vectorized the entire calculation and works with the state vector itself rather than a list of indices. In Figure 3.2 we plot the computation time required for each improvement of the op_on_state function. In Listing 3.1 we show our Python implementation of this algorithm for the case of L qubits. Next we comment on this code line by line.



Figure 3.2 Time scaling of algorithm for efficient local operator application. Tests were done on three version of the algorithm using a 4th generation Intel Core i7-4700MQ Processor. V0 labels version zero, the big matrix method; V1 labels version one, which removes the need for padding with identities; and V2 labels version two, which vectorizes the calculation done in version one. The connecting lines are a guide to the eye. The computation time reported here is for the application of a three-site-wide operator, analogous to $U_S^{\text{MODE}}(V)$, to a set of three qubits in a lattice of size L. Since a single QECA iteration requires L such applications we can estimate the computation time for simulating an iteration for a system size of L. For example, it takes about 25 seconds to simulate one iteration of an 25-site QECA.

The first line imports numpy, the only package necessary for this function. Next, in line 3, we define the function's name and inputs. The argument A is an *n*-site operator, js is a list of *n* sites onto which we will apply A, and state is the matrix representation of the system's state vector. Lines 4 and 5 compute the length of the lattice and the number of sites our

operator will act on. In line 6, we define ds which is a list of the local dimensions for each of our subsystems (all 2's for a lattice of qubits). Lines 7 and 8 compute the dimension of our *n* sites of interest, and the dimension of our entire Hilbert space. Then, in line 9, we compute the site indices which are to be unaffected by the local update (the "rest" of the lattice). In line 10, we concatenate **rest** with **js** to create a list of all the site indices but ordered such that the sites we are interested in are at the end of the list. Lines 11, 12, and 13 are really a single Python command, but with line breaks inserted for clarity. This one command is a major factor in what allows us to efficiently simulate with up to 27 sites, so it is work breaking down.

We begin with our current state, stored as a vector of length dL, which we reshape into an L-nested array. This is an L-index object. We then rearrange these L indices using ordering and the transpose function. This operation arranges the components of state into the correct groupings given the supplied js. We're now at line 12 where we do another reshaping of state's components, transforming it into a list of column vectors, each of the correct size and grouping to be right multiplied by A. The Numpy command dot is a vectorized dot product, meaning it will apply A to each column vector in our list. Once entries of state have been updated, we reshape back into an L-nested array. Next, at line 13, we unscramble the original transpose by transposing with respect to the argsort of our input ordering. The Numpy function argsort returns a list of indices which sort the input list in ascending order, in this case, ordering. Finally, we reshape back into the standard 1D shape of the state vector and set the net result to the variable new_state. The method is complete when **new_state** is returned in line 15. The generalization to arbitrary local dimension is done by allowing the user to input a list of local dimensions which are then used to calculate the dimension of the entire Hilbert space and the Hilbert space of the sites which we are operating on.

We've highlighted important considerations for the numerical implementation of QECA and described our key algorithm for time evolution. In the next section we will describe our Listing 3.1 Python code for efficient application of a local operator. This is the qubitspecific implementation of version two of op_on_state. The computation time of this algorithm is benchmarked against older versions in Figure 3.2. This algorithm is not only useful for the exact simulation of QECA but also for the approximate time evolution of Hamiltonian-based quantum dynamics via the Trotter expansion.

```
3.1
    import numpy as np
3.2
3.3
    def op_on_state(A, js, state):
         L = int(log(len(state), 2))
3.4
3.5
         n = len(js)
3.6
         ds = [2] * L
3.7
         dn = 2**n
         dL = 2 * * L
3.8
3.9
         rest = np.setdiff1d(np.arange(L), js)
3.10
         ordering = list(rest) + list(js)
3.11
         new_state = state.reshape(ds).transpose(ordering) \setminus
3.12
                   . reshape(dL/dn, dn).dot(A).reshape(ds) 
3.13
                   . transpose (np. argsort (ordering)). reshape (dL)
3.14
3.15
         return new_state
```

use of high performance computing facilities.

3.3 High performance computing for quantum elementary cellular automata

Our simulations were performed on the Colorado School of Mines cluster supercomputer known as Mio. The computer is a collections of nodes, each with a number of cores. Computations may be accelerated on these sort of machines by dividing a computation into parallelizable tasks. Memory is shared between cores of a node while each node has its own memory bank. A challenge of parallel programming is to avoid simultaneous reading and writing to the shared memory of a core, which could result in a race condition, while also allowing a single computation to span the distributed memory of several nodes [74]. This challenge is often faced using the Message Passing Interface (MPI) library, which provides programmers with a cross-platform set of tools for dealing with both shared and distributed memory in their computations [75]. The parallelism employed in our QECA studies is to run each simulation, all of which are completely independent of one another, simultaneously on the cores of several nodes. Since each task is independent, minimal message passing is required and thus this is a basic use case of MPI.

Mio utilizes an Intel x86 instruction set architecture, which is a set of instructions for dealing with native data types, low-level operations for registers, addressing modes, memory architecture, interrupt and exception handling, and external I/O [76]. As such, the processors used in Mio are all Intel-based. In our research, we specifically made use of eight nodes. Two of the nodes each have 20 cores operating at 2.70 gigahertz with 64 gigabytes of shared memory per node. The other six nodes each have 12 cores operating at 2.93 gigahertz with 24 gigabytes of shared memory per node. Combined, there are 112 cores, each of which can run one independent QECA simulation. While elementary compared to what is possible with MPI, our parallelization allows us to run more than 100 QECA simulations in the same amount of time that a serial use of our code would complete just one. In next chapter, we will take advantage of our ability to quickly run many QECA simulations to characterize the broad average properties of QECA evolution.

CHAPTER 4 BROAD ANALYSIS

with many qeca parameters which can be varied and many measures to apply to each simulation, we first seek a coarse grained picture of what qeca are capable of. to do this we will consider the spacetime averages of the measures \lceil, \rfloor, \dagger , and s^{vn} for a set of over 10,000 simulations. in this chapter, we describe the simulation parameters used to generate this data set and examine how the simulations distribute themselves along the axes of these measures. for context, the same measures are computed for a few well-characterized states from quantum information theory as well as random quantum states.

4.1 A mesoscopically large data set

all possible combinations of the following parameters are simulated:

$$L \in \{11, 14, 17, 20\} \tag{4.1}$$

$$S \in [1, 15] \tag{4.2}$$

$$V = HP(\theta) \text{ with } \theta \in [0^{\circ}, 90^{\circ}] \text{ in } 15^{\circ} \text{ increments}$$

$$(4.3)$$

 $MODE \in \{SWP, BLK, ALT\}$ (4.4)

for T = 1000 iterations and two classes of initial conditions, low density Fock states and well-characterized entangled states. By Fock state we are referring to the separable class of states corresponding to classical bit strings i.e., no super position in the computational basis. The given range of system sizes was selected because it spans nine sites, which is two powers of the neighborhood size. All rules are simulated except for rule 0 because, as can be see from Eqs. (2.59) and (2.60), it is the identity rule. Our choice of $V = HP(\theta)$ is motivated by the ability of the Hadamard gate to introduce local superposition, which can be visualized on the Bloch sphere as describe in Section 2.3.2. Additionally, the phase gate makes it possible to test the sensitivity of QECA dynamics to phase effects. To test the effect of local update ordering, we also simulate all three update modes defined in Section 2.5.

Four low density Fock states, enumerated

1. $|0...010...0\rangle$ 2. $|0...110...0\rangle$ 3. $|0...101...0\rangle$ 4. $|0...111...0\rangle$

are each simulated for every combination of simulation parameters given above. These Fock states are chosen because they correspond to the four unique neighborhood configurations. Since the states $|0...100...0\rangle$ and $|0...001...0\rangle$ are equivalent to the first Fock state in the above enumeration up to a translation, they are not considered unique. The same goes for the state $|0...011...0\rangle$ in relation to the second Fock state in the above enumeration. In total, four lattice lengths, 15 rules, seven phase gate angles, three update modes, and four initial conditions leads to $4 \cdot 15 \cdot 7 \cdot 3 \cdot 4 = 5,040$ Fock state simulations.

The six entangled states we simulate are given by

1. $|GHZ\rangle$ 2. $|W\rangle$ 3. $|0...0\rangle \otimes |\psi_+\rangle \otimes |0...0\rangle$ 4. $|0...0\rangle \otimes |\psi_-\rangle \otimes |0...0\rangle$ 5. $|0...0\rangle \otimes |\phi_+\rangle \otimes |0...0\rangle$ 6. $|0...0\rangle \otimes |\phi_-\rangle \otimes |0...0\rangle$

where $|GHZ\rangle$ and $|W\rangle$ are the GHZ and W states defined in Eqs. (2.51) and (2.52), respectively, and $|\psi_{\pm}\rangle$ and $|\phi_{\pm}\rangle$ are the four Bell states defined in Eq. (2.50). Thus, there are a total of 7,560 initially entangled simulations. Combined, this makes for 12,600 simulations ran for this study. At order of 10^4 , This isn't quite *big data*, but is instead what we call *mesoscopic data*. If one was willing, one could spend two minutes analyzing the results of each simulation so that, assuming a 40 hour work week, one could view each simulation in 10.5 weeks. Instead of this, we will automatically analyze simulations and bin them based on their average value of von Neumann entropy and network measures on the mutual information adjacency matrices.

Before analyzing the average broad structure of QECA dynamics, it is helpful to build our intuition for how a rule numbers affect QECA dynamics in a spatiotemporally resolved way. To this end, consider the 15 nontrivial rules evolving from a centered localized excitation of the form given as the first Fock state initial condition above. In Figure 4.1 we plot $\langle \sigma_j^z(t) \rangle$ for each site j and iteration t with L = 21 and T = 60. Additionally, we have set $V = HP(0^\circ)$, MODE = ALT, and allowed S to vary from 1 to 15. A system size of L = 21, or indeed any odd numer, makes for symmetric dynamics given the centered localized excitation initial condition. The expectation value of σ_j^z is bound between 1 and -1 and is equal to 1 (-1) if site j is in the basis state $|0\rangle$ ($|1\rangle$). Similarly, in Figure 4.2, we show the von Neumann entropy for the same set of simulation parameters. Clear symmetries with respect to rule number are apparent in Figure 4.1 and Figure 4.2. For example, rule 2 is the mirrored version of rule 4, and rule 6 appears symmetric and shows features common to rules 2 and 4.

The relative behavior of rules 2, 4, and 6 is a consequence of how the binary expansion of rule S informs the application of V to a site conditioned on that site's neighbors. The following analysis of these three rules is a direct application of the QECA numbering system defined in Section 2.5 and exemplified in Table 2.3. The binary expansion of 2 is 0010. Recall that each nonzero digit of this expansion encodes which configuration of neighbors results in an application of V. The second least significant bit is nonzero, and the binary expansion of that bit's significance, enumerated from zero, is 01. From the binary expansion of the nonzero digit's significance, we deduce that rule 2 applies V to a site conditioned
on that site's left neighbor neighbor being $|0\rangle$ and its right neighbor being $|1\rangle$. We find exactly the opposite recipe in rule 4, which expands to 0100. The only nonzero bit has significance 2, or 10 in binary. Thus, in rule 4, V is applied based on the left neighbor being $|1\rangle$ and the right neighbor being $|0\rangle$. To complete the example, consider rule 6 which has the binary expansion 0110. Since the nonzero elements of this expansion are the same two which appeared in rules 2 and 4, we say that rule 6 is the symmetrized version of rules 2 and 4. Combining what we already know about rules 2 and 4, we immediately realize that rule 6 applies V conditioned on the left and right neighbor being in opposite basis states. Similar symmetry triples can be formed with the rest of the rules, which we summarize in Table 4.1. The 11 unique dynamical structures observed in Figure 4.1 and Figure 4.2 come from seven symmetric rules and four unique asymmetric rules. The remaining four rules are equivalent to the first four asymmetric rules up to a reflection.

Table 4.1 Pairing QECA rules by symmetry. S^A and S^B are asymmetric partners, meaning that, for symmetric initial conditions, they are equivalent to each other up to spatial reflections. S^C is the symmetrized version of rules S^A and S^B . The subscript on S is either 2 or 10 and denotes the base of the rules representation. The rules labeled under S^A have an asymmetry in the application of V to sites with a $|0\rangle$ left neighbor and a $|1\rangle$ right neighbor. The rules labeled under S^B have an asymmetry in the application of V to sites with a $|1\rangle$ left neighbor and a $|0\rangle$ right neighbor. The states labeled S^C symmetrically apply V to sites with neighbors in opposite basis states. Additionally, rules 1, 8, and 9, not shown, are all symmetric and don't have asymmetric partners in the sense described here.

S^{A}_{10}	S_2^A ,	S_{10}^{B}	S_2^B	S_{10}^{C}	S_2^C
2	0010	4	0100	6	0110
3	0011	5	0101	7	0111
10	1010	12	1100	14	1110
11	1011	13	1101	15	1111

Our considerations thus far have helped build our intuition for how the QECA rule number affects its dynamics as observed in local expectation values and von Neumann entropy. We are almost ready to examine how our mesoscopically large data set is broadly characterized by entropy and network measure calculations. However, we will first calculate network measures on a few well-characterized quantum states so we may better interpret the results



Figure 4.1 Visualizing QECA dynamics with expectation values. Spacetime grids of $\langle \sigma_j^z \rangle$ for 15 different ECA rules, each initiated by a centered local excitation. Overall, we see 11 unique dynamical structures because rules 2, 3, 10, and 11 are mirrored version of rules 4, 5, 12, and 13, respectively. As an example of the variability in the observed dynamical structures, notice how the initial excitation may be be quickly dissipated into the lattice as with rule rule 7, coherently transferred to either end as with rule 6, or something in-between as with rule 14.



Figure 4.2 Visualizing QECA dynamics with von Neumann entropy. Spacetime grids of $s^{vN}(\rho_j)$ for 15 different rules each initiated by a centered local excitation. Comparing to Figure 4.1, we see that entropy (and thus entanglement) tends to follow the initial excitation, with the exception being rule 15 which generates no entanglement. These diagrams demonstrate that QECA are capable of generating diverse patterns of entanglement growth from a separable initial condition.

of our broad analysis.

4.2 Network measures for common entangled states

The motivation for computing mutual information network measures for a few wellcharacterized entangled states is twofold. First, such calculations allow us to intuit the structure of connectivity measured by the network measures. Second, it serves as a sanity check for our numerics by comparing to analytic results. In this section we will derive \mathcal{D} , \mathcal{C} and \mathcal{Y} for $|GHZ\rangle$, $|W\rangle$, a localized singlet, and an array of singlets for a lattice of length L. It is convenient to note that Eqs. (2.1), (2.2), and (2.4) imply that, for a constant adjacency matrix $\mathcal{I}_{jk} = a$ for $j,k = 0, \ldots, L-1$, we have $\mathcal{D} = a$, $\mathcal{C} = a$, and $\mathcal{Y} = 1/(L-1)$. In the case of a constant adjacency matrix, we will drop the jk subscript.

Start by computing the mutual information adjacency matrix for $|\text{GHZ}\rangle$. Notice that the reduced density matrix of any site j is completely mixed, that is,

$$\rho_j^{\text{GHZ}} = \frac{1}{2} (|0\rangle \langle 0| + |1\rangle \langle 1|). \tag{4.5}$$

The reduced density matrix for any two sites j and k is given by

$$\rho_{jk}^{\text{GHZ}} = \frac{1}{2} (|00\rangle \langle 00| + |11\rangle \langle 11|), \qquad (4.6)$$

a separable mixed state. Using Eqs. (2.54) and (2.55), we conclude that the mutual information adjacency matrix is a constant $L \times L$ matrix $\mathcal{I}^{\text{GHZ}} = 1/2$, except for the diagonal which we always define to be zero. We then can immediately write $\mathcal{D} = 1/2$, $\mathcal{C} = 1/2$, and $\mathcal{Y} = 1/(L-1)$

Next, for $|W\rangle$ we compute the one and two site reduced density matrices to be

$$\rho_{j}^{W} = \frac{1}{L} \left(|1\rangle \langle 1| + (L-1) |0\rangle \langle 0| \right)$$
(4.7)

$$\rho_{jk}^{W} = \frac{1}{L} \left(|01\rangle \langle 01| + |01\rangle \langle 10| + |10\rangle \langle 01| + |10\rangle \langle 10| + (L-2) |00\rangle \langle 00| \right).$$
(4.8)

The entropies needed for \mathcal{I}_{jk}^W are again computed with Eq. (2.54), but this time we need to diagonalize the subspace perpendicular to $|11\rangle$. This gives the fierst three eigenvalues $\alpha_1 = 0$,

 $\alpha_2 = 2/L$, and $\alpha_3 = (L-1)/L$. Since $|11\rangle$ does not have support in ρ_{jk}^W , it contributes a zero eigenvalue. Finally, Eq. (2.55) gives the constant adjacency matrix

$$\mathcal{I}^{W} = \frac{1}{L} + \frac{1}{2}\log(L) + \left(\frac{L-2}{2L}\right)\log(L-2) - \frac{L-1}{L}\log(L-1)$$
(4.9)

where, as before, we have dropped the subscript jk because the right-hand side of Eq. (4.9) is a constant with respect to entries of the adjacency matrix. Thus, $\mathcal{D} = \mathcal{I}^W$, $\mathcal{C} = \mathcal{I}^W$, and $\mathcal{Y} = 1/(L-1)$.

Both $|\text{GHZ}\rangle$ and $|W\rangle$ are states with spatially homogeneous entanglement. Therefore, it is no surprise that they both form completely connected mutual information adjacency matrices. Let us now consider a simple quantum state with inhomogeneous entanglement, an isolated singlet $|0...0\rangle \otimes |\psi_-\rangle \otimes |0...0\rangle$. Suppose that the singlet is shared between sites j = a and k = b with $a \neq b$. Intuitively, the mutual information adjacency matrix is then $I_{jk} = 1$ if (j, k) = (a, b) or (b, a) and 0 otherwise. It follows that $[\mathcal{I}^2]_{jk} = 1$ if (j, k) = (a, a)or (b, b) and $[\mathcal{I}^3]_{jk} = [\mathcal{I}]_{jk}$. Then, we arrive at $\mathcal{D} = 2/(L^2 - L)$, $\mathcal{C} = 0$, and $\mathcal{Y} = 2/L$ where we have used $[\mathcal{I}^3]_{jk} = \mathcal{I}_{jk}$ in evaluating the clustering coefficient.

Finally, consider a 1D array of singlets $|\psi_{-}\rangle \otimes |\psi_{-}\rangle \otimes \cdots \otimes |\psi_{-}\rangle$. For convenience take L to be even. Since each qubit is a part of a singlet, we have $\mathcal{I}_{jk} = 1$ if j is even and k = j + 1 or j is odd and k = j - 1. Otherwise $\mathcal{I}_{jk} = 0$. Again, we have $[\mathcal{I}^3]_{jk} = [\mathcal{I}]_{jk}$ and after similar manipulations to the localized singlet case, we see $\mathcal{D} = 1/(L-1)$, $\mathcal{C} = 0$, and $\mathcal{Y} = 1$.

In Figure 4.3 we compare our analytics and numerics for \mathcal{D} , \mathcal{C} and \mathcal{Y} as a function of L for the states $|GHZ\rangle$, $|W\rangle$, a localized singlet, and an array of singlets. We also show these results with the network measures as mutually perpendicular axes in Figure 4.4. Additionally, in Figure 4.4 we show the results of network measures computed for a random vector in Hilbert space. For a each L, 300 random states were generated, on which network measures were computed. The average measure value for the 300 samples is what is shown in Figure 4.4, where the standard deviation of each measure is of the same order or smaller than the symbol size. Now that it is clear how the network measures behave for random and wellcharacterized entangled quantum states, we are ready to use these measures to characterize the average behavior of the mesoscopically large data set introduced at the beginning of this chapter.

4.3 Equilibrium measure values

Because they are a novel new tool, we would like to quantify the amount of information gained by considering network measures for the broad analysis of the mesocopically large data set of over 10^4 simulations. To this end, we perform a principal component analysis on the set of time averaged values of \mathcal{D} , \mathcal{C} , and \mathcal{Y} . The time averages are taken for the last 500 iterations, after an initial period of 500 iterations which is ignored to allow for transients to dissipate. All of these values can be thought of composing an $N \times 3$ scatter matrix Z, where N is the number of simulations for which we are computing averages, e.g., N = 5,040 for the Fock initial conditions. After shifting the column-wise mean of Z to zero, we compute the three orthonormal eigenvectors of the matrix

$$C = Z^T Z. (4.10)$$

We interpret C as a symmetric correlation matrix and its eigenvectors point in the direction of the greatest spread of Z when Z's rows are plotted on orthogonal axes of \mathcal{D} , \mathcal{C} , and \mathcal{Y} . These eigenvectors are then the *principal components* of Z. For the Fock initial conditions, we find the three principal components to be

$$v_1 = 0.10482173\mathcal{D} + 0.98234926\mathcal{C} - 0.15492689\mathcal{Y} \tag{4.11}$$

$$v_2 = 0.41855966\mathcal{D} - 0.1848939\mathcal{C} - 0.88916931\mathcal{Y}$$
(4.12)

$$v_3 = 0.90211985\mathcal{D} - 0.02835811\mathcal{C} + 0.43055267\mathcal{Y}.$$
(4.13)

In Figure 4.5 we plot the scatter matrix Z and its three principal components for the Fock initial conditions. Similarly, the principal component analysis for the entangled initial conditions yields



Figure 4.3 Network measures of well-characterized entangled states. Agreement between numerics (circles) and analytics (solid black) displays a maximum absolute error on the order of 10^{-15} . Notice that the localized singlet is a decaying function of disparity because, as system size increases, the adjacency matrix approaches the uniform null network. Meanwhile, the singlet array is seen to be maximally disparate because each each node in the adjacency matrix is connected to exactly one other node, independent of system size, leading to disparate backbone-like structure.



Figure 4.4 Network measures for well-characterized entangled and random states scaling with system size L. Notice how all of these states remain near the limits of the measures, except for $|GHZ\rangle$ which bisects the range of \mathcal{D} and \mathcal{C} and the singlet array which saturates \mathcal{Y} . The similarly small magnitude of network measures for $|GHZ\rangle$, $|W\rangle$, and random states implies that larger values for network measures describe quantum states which are neither random nor structured like these well-characterized quantum states.

$$v_1 = 0.47691937\mathcal{D} + 0.87792771\mathcal{C} - 0.04231838\mathcal{Y}$$
(4.14)

$$v_2 = 0.87798586\mathcal{D} - 0.47359428\mathcal{C} + 0.06963687\mathcal{Y} \tag{4.15}$$

$$v_3 = -0.0410944\mathcal{D} + 0.07036611\mathcal{C} + 0.9966744\mathcal{Y} \tag{4.16}$$

which are plotted in Figure 4.6. Notice that in both cases there is one v_i with a large \mathcal{D} component, another with a large \mathcal{C} component, and a third with a large \mathcal{Y} component, meaning each of the three network measures is revealing unique information about the broad structure of our QECA simulations. An exception to this observation is seen in Eqs. (4.11) and (4.12) since both have \mathcal{D} and \mathcal{Y} components which are comparable. This implies that \mathcal{D} and \mathcal{Y} reveal redundant information about the quantum state of QECA evolving from an initial Fock state.

Next, in addition to \mathcal{D} , \mathcal{C} , \mathcal{Y} , we consider $s^{vN}(\rho_j)$. This lets us reduce each simulation to an ordered-quadruple which we visualize on scatter plots of six possible 2D slices. For the Fock initial conditions, these six slices are shown in Figure 4.7 where we've colored the scatter points by L and Figure 4.8 where the scatter points are colored by S. In both



Figure 4.5 Principal component analysis for Fock state initial conditions. Each of the 5,040 simulations is reduced to three scalars, the averages of \mathcal{D} , \mathcal{C} , and \mathcal{Y} over the last 500 iterations of 1000 iteration simulations. The principal components given by Eqs. (4.11), (4.12) and (4.13) are plotted as v_1 in blue, v_2 in green, and v_3 in red. We have normalized by the max value seen for each measure for clarity.



Figure 4.6 Principal component analysis for the entangled initial conditions. The principal given by Eqs. (4.14), (4.15) and (4.16) are plotted as v_1 in blue, v_2 in green, and v_3 in red.

figures panel (c) shows a clear one-to-on trend between \mathcal{D} and \mathcal{C} . This trend is to be expected because denser networks are naturally more transitive. For both figures we also see a positive trend between \mathcal{D} and s^{vN} for $s^{vN} < 0.6$ and a negative trend for $s^{vN} > 0.6$ in panel (d). In Figure 4.8 rules 2 and 4 tend to cluster together, as do rules 10 and 12, because these rule pairs are asymmetric partners, as listed in Table 4.1.

In Figure 4.9 we show the frequency with which simulations fall into a binning of the axes determined by the six slices. Notice that most simulations average out to having relatively low values for all three of our complex network measures, though there are also many simulations which have network measures far different from those of the common entangled and random states seen in Figure 4.4.

Similarly, in Figure 4.10 we show the scatter plots of the entangled initial conditions colored by L. Observe in panel (c) the strong correlation between \mathcal{D} and \mathcal{C} which persists for larger magnitudes than seen with the Fock initial conditions. When the average network quantities are colored by rule number, as in Figure 4.11, we find in panel (c) the one-to-one correspondence between \mathcal{C} and \mathcal{D} is most strongly violated by rules 2, 4, 10, and 12. These rules are biased towards lower \mathcal{D} because of the large asymmetry inherent in their dynamics, visualized in e.g., Figure 4.1. Finally, in Figure 4.12 we show histograms of points falling into a binning of the axes given by the six slices for initially entangled initial conditions. Notice the average dynamics of initially entangled quantum states are best distinguished by the disparity and von Neumann entropy axes because there are more points spread over a larger area of this slice.

Overall, the network measures are larger for initially entangled initial conditions than for the Fock initial conditions. Additionally, disparity's dependence on L is the cause of of several clusters in Figure 4.10 panels (a) and (b) at about $\mathcal{Y} = 0.1$ and in panel (f) at about $\mathcal{Y} = 0.2$.

In this chapter we have seen how random and well-characterized quantum states appear on the axes of network density, clustering coefficient, and disparity. This was contrasted with the average value of these measures found in QECA dynamics. Comparing Figure 4.4 to e.g. Figure 4.11, it is clear that, on average QECA are capable of generating states which are neither random nor a well-characterized quantum state. In the next chapter, we will begin to unravel QECA dynamics using discrete Fourier transforms in one and two dimension.



Figure 4.7 Broad structure of QECA highlighting L dependence: Fock initial conditions. Six 2D slices of the long time average of 4 measures of QECA dynamics. Panels (a), (b), and (c) demonstrate the diversity of highly structured two point correlation as compared to Figure 4.4. Panels (d), (e) and (f) demonstrate the relationship between one and two point-entropic quantities. Network measures are derived from quantum mutual information, which depends on the two point von Neumann entropy, while the entropy of the vertical axes of (d), (e), and (f) are the average one-point entropy.



Figure 4.8 Broad structure of QECA highlighting S dependence: Fock initial conditions. The data shown here is identical to that of Figure 4.7 but with points colored by S to demonstrate the clustering of values for simulations with the same rule number.



Figure 4.9 Diversity of QECA broad structure: Fock initial conditions. Histograms showing a 20×20 binning for the six slices of four measures. The highest density of simulations is found near the origin of these slices which means these simulations are, on average, exhibiting a network structure like $|W\rangle$ or random states.



Figure 4.10 Broad structure of QECA highlighting L dependence: entangled initial conditions. Six 2D slices of the long time average of 4 measures on QECA dynamics. We find similar structures to the Fock initial conditions but across a wider range of observed for the measures.



Figure 4.11 Broad structure of QECA highlighting S dependence: entangled initial conditions.



Figure 4.12 Diversity of QECA broad structure: entangled initial conditions. Histograms showing a 20×20 binning for the six slices of four measures. As seen in ??, highest density of simulations is found near the origin of meaning these simulations are, on average, exhibiting a network structure like $|W\rangle$ or random states.

CHAPTER 5

COMPLEXITY DYNAMICS IN THE FREQUENCY DOMAIN

In this chapter we will investigate QECA dynamics using Fourier analysis. Doing so uncovers a rich structure of QECA dynamics missed by the average analysis presented in 4. A one-dimensional discrete Fourier transform is applied to the network measures \mathcal{D} , \mathcal{C} , and \mathcal{Y} as well as the spatial average of the expectation values $\langle \sigma_j^z(t) \rangle$, defined as

$$\langle \sigma^z(t) \rangle = \frac{1}{L} \sum_{j=0}^{L-1} \left\langle \sigma_j^z(t) \right\rangle.$$
(5.1)

Since the network measures quantify complexity in terms of connectivity, one of the nine axes of complexity outlined in Section 2.1, the Fourier transforms of network measures describes complexity dynamics. Significant spectral features present in the one dimension transforms are found as peaks above an estimated a red noise spectrum. Similarly, a two-dimensional discrete Fourier transform is applied to the spacetime grid of expectation values $\langle \sigma_j^z(t) \rangle$. In both the one and two dimensional case, our primary focus will be on the effects of rule number on the observed spectra for otherwise identical simulations. Before showing the results of this chapter, a few important definitions and properties of discrete Fourier transforms are recalled.

5.1 Discrete Fourier transforms

The fundamental idea underlying Fourier analysis is that single-frequency signals, e.g. complex exponentials, with different frequencies may be used as an orthonormal basis for constructing an arbitrary signal. The Fourier transform of a signal reveals the relative weights, or amplitudes, with which each single-frequency component present in that signal. In general, it takes a continuum of frequencies to reproduce an arbitrary signal. In practice, one often uses a *discrete Fourier transform* to approximate the input signal with a finite number of single-frequency components. In this way, if the input signal is a measurement

of some process in a physical system, the Fourier transform of that signal reveals the time scales on which that process is occurring.

Since all of the signals we intend to transform are discrete, we will refer to the discrete Fourier transform as just the Fourier transform for brevity. Moreover, we will be using the following definition for the Fourier transform of a signal a of length T which is a function of the discrete variable t

$$A(f) = \sum_{t=0}^{T-1} a(t) \exp\left(-2\pi i \frac{tf}{T}\right) \quad \text{for } t = 0, 1, \dots, T-1$$
 (5.2)

where A(f) is the amplitude assigned to the discrete reciprocal space variable f and i is the imaginary unit. The inverse transform is then

$$a(t) = \frac{1}{T} \sum_{f=0}^{T-1} A(f) \exp\left(2\pi i \frac{tf}{T}\right) \quad \text{for } f = 0, 1, \dots, T-1.$$
(5.3)

Analogously, in two dimensions the transform and inverse transform pair is

$$A(f,k) = \sum_{t=0}^{T-1} \sum_{x=0}^{L-1} a(t,x) \exp\left(-2\pi i \left[\frac{tf}{T} + \frac{xk}{L}\right]\right)$$
(5.4)

$$a(t,x) = \frac{1}{TL} \sum_{f=0}^{T-1} \sum_{k=0}^{L-1} A(f,k) \exp\left(2\pi i \left[\frac{tf}{T} + \frac{xk}{L}\right]\right).$$
(5.5)

Additionally, for a real-valued signal, the transformed signal is symmetric with respect to positive and negative frequencies, though it is possibly complex-valued. For this reason, our plots of a signal's Fourier transform show the power spectrum

$$\mathcal{F}(a(t,x)) \equiv |A(f,k)|^2 \tag{5.6}$$

for only positive frequencies.

The minimum and maximum frequencies which can be resolved in a Fourier transform are determined by the sampling rate with which the signal was obtained. Since QECA are updated through time in discrete iterations, our sampling rate is one sample per iteration. Since at least two samples are required to resolve a periodic signal, the highest resolvable frequency is 0.5 cycles per iteration, known as the *Nyquist frequency*. Similarly, the lowest resolvable frequency is zero cycles per iteration, which is the average value of the signal and is sometimes called the DC-level. The overall resolution of the Fourier transform is determined by the number of samples in the original signal and is given by 1/T cycles per iteration where T is the number of samples in the original signal. In the next section, we use Fourier transforms to determine the frequencies of dominant processes in QECA dynamics.

5.2 Spectral features of one-dimensional measures

The complex network measures \mathcal{D} , \mathcal{C} , and \mathcal{Y} are scalar-valued functions at each iteration. Along with the average expectation value of the Pauli z operator defined in Eq. (5.1), we have four one-dimensional measures to compute power spectra for.

To compare the frequencies of dominant processes between different rule numbers, the noise floor is estimated for all the Fourier transforms we compute. Then, peaks which are significant at a > 95% confidence level with respect to this noise floor are deemed significant and collected for comparison. The noise floor is estimated by fitting a *red noise* spectrum to the power spectrum of each measure. Red noise has zero mean, constant variance, and is serially correlated in time [77]. The degree to which red noise is correlated in time is given by a parameter called *redness*, denoted r. Since white noise has zero mean, constant variance, and variance, and is uncorrelated in time, red noise is like white noise (also called Gaussian or normal noise) but with a short-term memory. While the power spectrum of white noise is equally distributed across all frequencies, red noise is biased towards low frequencies, hence its name.

The noise floor of the power spectrum of a signal a(t) is estimated by

$$P_{\rm rn}(f;r) = P_0 \frac{1 - r^2}{1 - 2r\cos(2\pi f) + r^2}$$
(5.7)

where the redness r is estimated by the autocorrelation at lag one of the input signal and the normalization factor P_0 is chosen so that the red noise power spectrum has the same total power as the power spectrum of the input signal. The autocorrelation at lag m of a signal a(t) with mean μ is given by

$$\frac{\sum_{t} (a(t) - \mu)(a(t+m) - \mu)}{\sum_{t} (a(t) - \mu)^2}.$$
(5.8)

where the t is summations are from 0 to T - 1.

Next, treat the red noise spectrum as a null hypotheses for the presence of spectral features. That is, we reject the null hypotheses that the input signal's power spectrum is nothing more than red noise if spectral features rise above the estimated noise floor. To make a more statistically rigorous statement, compute a 95% confidence red noise spectrum by multiplying Eq. (5.7) by χ^2_2 , the chi-squared distribution with two degrees of freedom corresponding to the desired confidence level. For a 95% confidence level, we use χ^2_2 at a p-value of 0.05 which has the approximate value 5.991 [78].

In Figure 5.1 we show the power spectrum of each measure for an L = 17 site simulation of rule 14 with $V = HP(\theta)$, MODE=ALT for T = 1000 iterations initiated with a centered localized excitation of the form $|0...010...0\rangle$. In this figure and throughout the remainder of this analysis, the first 300 iterations are removed before transforming the signal to remove transient effects without a major loss of spectral resolution. Additionally, to aid in the task of peak finding, we smooth the power spectrum with a five-point moving average, then reject peaks found below the 95% confidence level. The results of simulations with rules 4 and 6 and otherwise identical simulation parameters to those stated above are shown in Figure 5.2 and Figure 5.3, respectively. Observe that no significant spectral features are found in the power spectrum for rule 14. For rule 4, the power spectrum of the average expectation value of the Pauli z operator is found to be comparatively cleaner than the other measures, though significant spectral features are found for each measure. Rule 6 yields power spectra which all show prominent spectral features in the same vicinity as one another.

The results of similar analyses under the same simulation parameters but for rules 1 through 15 are summarized in Figure 5.4. In this figure, the horizontal axis is partitioned by rule number and the vertical axis gives the frequency of significant spectral features found in



Figure 5.1 Spectral features of rule 14 present in the power spectrum of network measures and the average expectation value of the Pauli z operator. The solid blue line is the raw red noise spectrum and the dashed blue line is the 95% confidence red noise spectrum. Since no significant spectral features are found, we may not reject the red noise null hypothesis and further analysis would be required to claim the power spectrum or rule 14 only exhibits red noise.



Figure 5.2 Spectral features of rule 4 present in the power spectrum of network measures and the average expectation value of the Pauli z operator. The solid blue line is the raw red noise spectrum and the dashed blue line is the 95% confidence red noise spectrum. The average expectation value of the Pauli z operator yields a power spectrum quite different in character than the network measures, though each have significant spectral features in common.



Figure 5.3 Spectral features of rule 6 present in the power spectrum of network measures and the average expectation value of the Pauli z operator. The solid blue line is the raw red noise spectrum and the dashed blue line is the 95% confidence red noise spectrum.

the power spectra of the four measures under consideration. Rules for which no significant spectral features were found, like rule 14, have been omitted. For reference, the frequency of magnitude 1/L is also shown. For a lattice of size L, there is a natural frequency one may expect to see significant features assuming the initial excitation travels at a constant speed v. If one takes this speed to be v = 1 site per iteration, the natural frequency we are referring to has a magnitude of 1/L cycles per iteration, which we will call the v = 1bouncing frequency. In Figure 5.4, we find that there are significant spectral features which tend to cluster just above the v = 1 bouncing frequency, suggesting transport at speeds greater than v = 1 site per iteration. Rules 6, 9, 10, and 12 show spectral features below the v = 1 bouncing frequency. Additionally, Notice that the symmetries in rule number discussed in Section 4.1 and summarized in Table 4.1 are recapitulated in Figure 5.4. That is, rules which yield mirrored dynamics, such as rules 2 and 4, display similar significant spectral features.

5.3 Inspection of two-dimensional transforms

By substituting Eq. (5.2) into Eq. (5.1) we can see that the Fourier transform of an average quantity is the average of the Fourier transforms of each quantity making up the average. It is possible that such an averaging procedure will obscure relevant structure in the frequency domain. To get a spatially resolved picture of the dynamics in the frequency domain, consider instead the two-dimensional transform of the spatially resolved expectation values $\langle \sigma_j^z(t) \rangle$. Using Eq. (5.5) we compute the power spectrum $\mathcal{F}(\langle \sigma_j^z(t) \rangle)$ as a function of spatial frequency, or wave number, k, which is dual to the site index j and the temporal frequency f, which is dual to the iteration number t. Thus, a two dimensional Fourier transform can be visualized as a reciprocal-space grid with f and k on mutually orthogonal axes. The relationship between f and k is often referred to as a dispersion relation. In Figure 5.5 we show the dispersion relation for rules 4, 6 and 14 simulated with $V = HP(0^{\circ})$, MODE=ALT for T = 1000 iterations and initiated with a centered localized excitation. Notice that rule 14, for which we could not reject the red noise null hypothesis in the one-dimensional



Figure 5.4 Summary of significant spectral features of the one dimensional power spectrum of network density, clustering coefficient, disparity, and the spatial average of expectation values of the Pauli z operator. The vertical dashed lines partition different rules. The horizontal dotted line is at a magnitude of 1/L and represents the frequency of processes occurring at the natural time scale induced by a lattice of finite size L assuming a constant velocity of one site per iteration, the v = 1 bouncing frequency. Rules 7, 8, 11, 13, and 14 were found to have no significant spectral features and thus are omitted here.

case, shows much more structure in the two dimensional Fourier transform.

In Figure 5.6, we show the dispersion relation for rule 1 for increasing phase gate angle, but with otherwise identical simulation parameters to those used in this chapter thus far. Observe the spatial period-doubled band structure at high temporal frequency. A similar dispersion relation is found for Bose-Einstein condensates in a periodic optical lattice [79, 80]. In our case, the period-doubled band is a decreasing function of phase gate angle. As phase gate angle increases, the period-doubled band approaches a low frequency continuum portion of the spectrum which is present at high wave number, independent of phase gate angle.

In this chapter we have supplemented our understanding of QECA dynamics with an analysis in the frequency domain. In Chapter 4 we found that the average value of network measures attained by QECA can be quite different from the values of network measures of both well-characterized and random quantum states. In this chapter we quantified the most significant frequencies in the complexity dynamics which give rise to the observed average values. In the next chapter, we will continue our investigation of QECA dynamics but with an emphasis on entanglement generation.



Figure 5.5 Two-dimensional power spectrum of rules 4, 6, and 14 shown in panels (a), (b), and (c), respectively, as the reciprocal-space grid of $\mathcal{F}(\langle \sigma_j^z(t) \rangle)$. For rule 4, the strong horizontal bands of constant f in panel (a), agree with the strong peaks observed in the average power spectrum of the expectation values of the Pauli z operator, shown in Figure 5.2. The linear dispersion of rule 14 apparent in panel (c) was hidden by the average picture presented in Figure 5.1. From panel (b), it appears that rule 6 shows a linear trend similar to rule 14 and lines of constant f similar to rule 4.



Figure 5.6 Two-dimensional power spectrum of rule 1 for $\theta = 0^{\circ}$, 45° and 90° in panels (a), (b), and (c), respectively. In all cases there is a continuum at low temporal frequency and high wave number. At high frequency we notice a spatial-period doubled band structure. The gap between the continuum and the spatial period-doubled band is a decreasing function of phase gate angle.

CHAPTER 6 THE APPROACH TO EQUILIBRIUM

We have seen how the long time averages of thousands of QECA simulations are distributed with respect to the various quantum measures. While this averaging procedure allowed us to get a broad picture of QECA, we would like a clearer picture of the entanglement dynamics which are underlying these averages. In this chapter we will investigate entanglement dynamics using bond entropy. Some QECA will show quick equilibration of entanglement while others remain dynamic. We will argue that the QECA which remain dynamic are exhibiting complexity in the sense of persistent dynamical macrostates. Specifically, these persistent dynamical macro states are quantum states exhibiting dynamical many-body entanglement, as quantified by the bond entropy.

6.1 Characterizing many body entanglement

Bond entropy is the von Neumann entropy of a bipartitioning of the lattice at cut $c = 0, \ldots L - 2$, where L is the length of the QECA lattice and the c^{th} cut splits the lattice into two sets of site indices $A = \{0, \ldots, c\}$ and $B = \{c + 1, \ldots, L - 1\}$. At each cut we need only compute the reduced density matrix and von Neumann entropy of the smaller of the two partitions, thanks to the Schmidt decomposition. Without loss of generality, take A to be the smaller bipartition at cut c. Then, the bond entropy is

$$s_c^{\text{bond}}(t) = s^{\text{vN}}(\rho_A(t)) \tag{6.1}$$

Even though the bond entropy is nothing more than the von Neumann entropy, we give it a unique name and symbol for brevity and to remind us it is a has a slightly different interpretation than the single-site von Neumann entropy. We normalize s_c^{bond} to lie between zero and one as $s_c^{\text{bond}}/\min(c+1, L-c)$ (recall that the von Neumann entropy of d qubits is largest for the maximally mixed state and has a value of d). Under this normalization, a bond entropy equal to one implies the entirety of the smaller half of the lattice is entangled with the rest of the lattice. Thus, the physical significance of the bond entropy is that it quantifies the entanglement between larger portions of the lattice in a spatially resolved way. That is, for cuts c = 0 and c = L - 2, the bond entropy is equivalent to the local von Neumann entropy of sites j = 0 and j = L - 1, respectively. Notice that the bond entropy for all cuts quickly becomes an expensive computation for large L, as it involves solving for the eigenvalues of L - 2 reduced density matrices, the largest of which is $2^{\lfloor L/2 \rfloor} \times 2^{\lfloor L/2 \rfloor}$. In Figure 6.1 we show the bond entropy for the first 60 iterations of rules 1 through 15 using MODE = ALT, $V = HP(0^{\circ})$, and L = 19 for the initial condition $|0 \dots 010 \dots 0\rangle$.

6.2 Iteration-wise deviation

For the purposes of this study, we will consider the entanglement in our QECA simulation to have equilibrated when its fluctuations from iteration to iteration are no longer trending positively or negatively. To this end, consider the iteration-wise difference of bond entropy given by

$$\Delta s^{\text{bond}}(t) = s_c^{\text{bond}}(t+1) - s_c^{\text{bond}}(t) \quad \text{for } c = 0, \dots L - 2.$$
 (6.2)

If an element of $\Delta s^{\text{bond}}(t)$ is positive (negative), entanglement has undergone a net increase (decrease). If we collect all of the iteration-wise deviations into a histogram we can get a rough picture of the entanglement dynamics in a particular simulation. A wide distribution of $\Delta s^{\text{bond}}(t)$ means that entanglement is changing nonuniformly from iteration to iteration, while a narrow distributions is indicative of fast-equilibrating entanglement. In Figure 6.2 we show the histograms of iteration-wise deviation of the bond entropy for rules 6, 7, 9, and 14 using MODE = ALT, $V = HP(0^{\circ})$, and L = 19 for the initial condition $|0 \dots 010 \dots 0\rangle$.

To better understand how different segments of iterations contribute to the aggregate binning of the iteration-wise bond entropy observed in Figure 6.2, we subdivide the dynamics into groups of τ iterations and compute the average of Δs^{bond} for each subdivision. In Figure 6.3 we show the results for $\tau = 19$ with rules 6, 7, 9, and 14 using MODE = ALT,



Figure 6.1 Bond entropy illustrating the structure and dynamics of many body entanglement in QECA. Bond entropy tends to be lower for cuts near the center of the lattice than for those at the edges, but a bond entropy greater than 0.5 in the center of the lattice implies many body entanglement involving at least L/4 sites. As such, we observe highly structured many body entanglement in most of these simulations.



Figure 6.2 Aggregate distribution of Δs^{bond} for 1000 iterations. Rule 7 generates more entanglement than it destroys while rules 6, 9, and 14 tend to create and destroy entanglement equally. Rules 6 and 9 have broad distributions and thus are not equilibrating quickly.

 $V = HP(\theta)$ with $\theta = 0^{\circ}$, 45°, and 90° and L = 19 for the initial condition $|0...010...0\rangle$. The choice of $\tau = 19$ was made because it is the same as the system size.

Using Figure 6.3 we identify rule 9 as a fragile persistent macrostate because introducing a nonzero phase gate drives Δs^{bond} to a value two orders of magnitude smaller than its value at $\theta = 0^{\circ}$. Meanwhile, Δs^{bond} remains within a single decade for S = 6 at all θ shown, meaning its dynamics are more robust to changes in phase gate. Comparing relative magnitudes of Δs^{bond} , we see that rules 6 and 9 typically remain more dynamic than rules 7 and 14.

Overall we conclude that, of rules 6, 7, 9, and 14 for $\theta = 0^{\circ}$, rule 7 exhibits the least dynamical many body entanglement. Additionally, rule 6 remains the most dynamical for nonzero θ . To summarize the results we've obtained for these four rules as well as to check the long time behavior of other rules, we plot the last 60 iterations (of 1000) of the entanglement dynamics first visualized in Figure 6.1. In Figure 6.4 and Figure 6.5 we show the late-time entanglement dynamics at $\theta = 0^{\circ}$ and $\theta = 90^{\circ}$, respectively. We conclude that rule 6 exhibits the most robust entanglement dynamics. Apparently, rule 1 also shows robust dynamical many body entanglement dynamics, but the overall level of entanglement is lower than that seen in rule 6. In the next chapter, we will take a closer look at the dynamics or rule six with a particular emphasis on its ability to transport initially localized excitations.



Figure 6.3 Average distribution of Δs^{bond} for 1000 iterations subdivided in groups of $\tau = 19$ iterations. Open circles are the data while connecting lines are a guide to the eye. All plots have been placed on the same vertical scale to highlight differences. Decaying curves describe a simulation's approach to equilibrium while constant, large values imply no equilibrium level of entanglement is being approached.



Figure 6.4 Examples of the late-time evolution of bond entropy for $\theta = 0^{\circ}$ show obvious dynamical many body entanglement for rules 6, and 9. Smaller fluctuations are also apparent in rules 1, 7, and 14.


Figure 6.5 Examples of the late-time evolution of bond entropy for $\theta = 90^{\circ}$ shows smoother fluctuations for all rules as compared to the $\theta = 0^{\circ}$ case, though rule 6 remains noticeably more dynamic than other rules.

CHAPTER 7 SPEED AND DIFFUSION RATE

In Section 4.1 we deduced rule S = 6 symmetrically applies V to site j conditioned on j's left and right neighbors being in opposite basis states. This rule can transport localized excitations across the lattice. In this chapter, we investigate the speed at which local excitations are transported, a quantity we call the speed of sound, a term often used in solid state physics for the group velocity of phonon excitations. Like the group velocity, our speed of sound is the speed with which information is propagated across the lattice (with high probability). We also investigate the rate at which the local excitation diffuses into the rest of the lattice, what we call the diffusion rate. Together, the speed of sound and diffusion rate describe a rule's transport properties. Our main focus will be on how these transport properties depend on the phase gate angle of V and the update mode. We will compare these results with transport properties observed in the classical version of rule 6, i.e. $V = \sigma^x$, which exhibits what we call the QECA's native transport properties. Our definitions of speed and diffusion rate are based on the first and second moments (respectively) of the probability of measuring the excitation at all sites for all iterations. We first turn to making these definitions.

7.1 Center and diffusion of probability

The initial condition for this analysis will be a single localized excitation at either end of the lattice. The localized excitation can be described as a single $|1\rangle$ qubit in an otherwise $|0\rangle$ lattice. For the left excitation, the initial state is written $|1\rangle \otimes |0\rangle^{\otimes L-1}$ while the right excitation is written $|0\rangle^{\otimes L-1} \otimes |1\rangle$.

The probability of measuring a 1 at site j and iteration t is given by $\text{Tr}(\rho_j(t)\hat{P}_1)$ where $\rho_j(t)$ is the reduced density matrix of site j at iteration t and \hat{P}_1 is the projector onto the subspace spanned by the $|1\rangle$ basis state. We will use the short hand $P_1(j,t)$ to denote this

probability spacetime grid. $P_1(j,t)$ can be thought of as a time series of spatial probability distributions for measuring a 1. The first moment of $P_1(j,t_0)$ at some iteration t_0 gives the average location for measuring a 1, making it a measure of the center of probability. Similarly, the second moment gives a width around the first moment in which a 1 will be found with high probability, a measure of the diffusion of probability. Let $\mu_{P_1}(t)$ and $\Delta_{P_1}(t)$ denote the first and second moment of $P_1(j,t)$. To first order, we may compute the speed of sound as the slope of a linear fit to $\mu_{P_1}(t)$ and the diffusion rate to be the slope of a linear fit to $\Delta_{P_1}(t)$. The fits are restricted to the set of iterations prior to impact of $\mu_{P_1}(t)$ with the opposite end of the lattice.

7.2 Native and emergent transport

Before describing the main result of this chapter, let's look at a few examples of the excitation propagation in rule 6. First, for a classical QECA, which we define as one with $V = \sigma^x$, we can deduce how the update mode (SWP, BLK, or ALT) affects the excitation's propagation speed. The classical speeds are the same as those deduced from the circuit diagrams given at the end of Section 2.5 and thus display the bounds of the speed of sound. In Figure 7.1 we plot $P_1(j,t)$ for the SWP, BLK and ALT modes. Notice that the classical QECA display no diffusion. Of these examples, the maximum speed is observed for rightward propagation with MODE = SWP and is L sites/iteration while the minimum speed is observed to be 1 site/iteration for leftward propagation, also appearing with MODE = SWP. In the BLK scheme, the speeds are 3 sites/iteration rightward and about 1.5 sites/iteration leftward. The ALT mode exhibits propagation speeds of 2 sites/iteration in both directions. All three update modes have the same average speed of 2L/(L+1) sites/iteration. Since the classical version of rule 6 exhibits the maximal speed of sound and the minimum diffusion rate we say the transport properties are ideal and particle like. Furthermore, since the speed of sound for each mode agrees with what can be inferred from each mode's circuit diagram, the classical QECA may be thought of as defining the *native* transport properties.



Figure 7.1 Native rightward and leftward transport in rule 6 can be seen for the SWP, BLK, and ALT modes when using $V = \sigma^x$.

It is interesting that the transport properties of rule 6 depend on the choice of V. Moreover, the transport properties can be coarsely controlled by introducing a nonzero phase gate angle. In Figure 7.2, Figure 7.4, and Figure 7.3 we show the probability spacetime grids for rule 6, and MODE =SWP, BLK, and ALT, respectively, with examples of $V = HP(\theta)$ for $\theta = 0^{\circ}$, 45°, and 90°. Qualitatively it is clear that as θ increases, both speed of sound and diffusion rate decrease. This is a clear divergence from the native transport properties in Figure 7.1, though the relative left-right and right-left transport asymmetry in SWP and BLK is preserved. This new behaviors are interpreted as emergent transport features, signaling some level of complexity. That is, introducing a decisively quantum V (by which we are referring to the ability of $HP(\theta)$ to introduce new local superpositions with each application), we observe new transport features including a non-zero diffusion rate and a slower speed of sound. Perhaps more striking is the ghostly trail with a high speed of sound and high diffusion rate observable for large θ . This *phantom particle* travels with the same speed of sound as the primary excitation when simulated with $\theta = 0$.



Figure 7.2 Emergent rightward and leftward transport of rule 6 with MODE = SWP with $V = HP(\theta)$. Here we show $\theta = 0^{\circ}, 45^{\circ}, 90^{\circ}$.

7.3 Transport properties and phase gate angle

In this section we will outline a procedure for quantitatively measuring the transport properties of rule 6. For this study, we use a system size of L = 21 and $\theta \in [0,90^{\circ}]$ in 5° increments. The phantom trajectory makes $P_1(j, t_0)$ bimodal (has two peaks) for most θ . We will quantify the transport properties of the primary trajectory because it changes with θ . To do this, we must have a way of distinguishing two peaks so that we can ignore the phantom trajectory. We do this by applying a 2-mode Gaussian mixture model to each iteration of $P_1(j, t)$. This allows us to estimate two pairs of transport properties $\{\mu_{P_1}^{(1)}(t), \Delta_{P_1}^{(1)}(t)\}$ and $\{\mu_{P_1}^{(2)}(t), \Delta_{P_1}^{(2)}(2)\}$ where the superscripts (1) and (2) denote the primary and phantom trajectories, respectively. In practice, one has to track which pair relates to which trajectory from iteration to iteration. This can be done by first initializing the (1) index to be the peak with the highest vaue of $P_1(j, 0)$. Then, for iteration t = 2, we set the (1)-index pair to be the pair for which $\mu_{P_1}(t = 2)$ is closest to $\mu_{P_1}(t = 1)$.



Figure 7.3 Emergent rightward and leftward transport of rule 6 for MODE = BLK with $V = HP(\theta)$. Here we show $\theta = 0^{\circ}, 45^{\circ}, 90^{\circ}$.

This process can be iterated to keep track of which pair of moments belongs to which trajectory until the pairs intersect. Instead of passing through each other as is apparent in e.g., Figure 7.4, the two peaks are seen to "bounce" off of one another. This computational artifact is due to the fact that at the iteration of the intersection, t_{int} , $P(j, t_{\text{int}})$ isn't bimodal, and hence a 2-mode Gaussian mixture model is a poor hypothesis. To remedy this situation, we set an interaction radius inside of which, the results of the 2-mode Gaussian mixture model are averaged, yielding the single pair of moments $\{\mu_{P_1}(t_{\text{int}}), \Delta_{P_1}(t_{\text{int}})\}$. We found the quantity $\frac{1}{2}(\Delta_{P_1}^{(1)}(t) + \Delta^{(2)}(t))$ to provide an effective definition for the interaction radius using the proximity measure $|\mu_{P_1}^{(1)} - \mu_{P_1}^{(2)}|$. This technique solves the bouncing problem and also allows us to effectively measure the transport properties for simulations with low θ . In Figure 7.5 we show the results of our 2-mode Gaussian mixture model for tracking the two trajectories in the vicinity of their interaction.



Figure 7.4 Emergent rightward and leftward transport of rule 6 for MODE = ALT with $V = HP(\theta)$. Here we show $\theta = 0^{\circ}, 45^{\circ}, 90^{\circ}$.

The final results detailing the transport properties of rule 6 are shown in Figure 7.8. Near $\theta = 45^{\circ}$ there is an inflection point in the speeds of sound for both left and right moving particles and for all modes. Thus near $\theta = 45^{\circ}$ the speed of sound is most sensitive to perturbations in θ . As expected from the observations made with $V = \sigma^x$, SWP possesses the largest variability between leftward and rightward speeds of sound, followed by BLK, and finally ALT which is completely symmetric transport properties. However, BLK is more similar to ALT than it is to SWP. That is BLK is shows more symmetric transport properties than SWP.

Diffusion rate peaks near $\theta = 25^{\circ}$ then falls rapidly. Beyond $\theta = 55^{\circ}$ diffusion is nearly zero. Thus, here the primary excitation propagates with soliton-like qualities in that it does not diffuse after intersection with the phantom particle on impact with the end of the lattice. The character of the diffusion rate can be understood by examining the separation of the primary and phantom trajectories. For small θ , the two trajectories have significant overlap,



Figure 7.5 Two-mode Gaussian mixture model used for peak and width finding of the two trajectories under ALT update mode. The raw data is plotted in blue, the net mixture model is plotted in green, and the mixture components corresponding to the main and phantom trajectories are plotted in solid and dashed black, respectively. Rightward propagation is plotted in panel (a), and leftward propagation is plotted in (b).

meaning the highly diffusive phantom trajectory is inseparable from the soliton-like primary trajectory. This overlap also poses fitting challenges when using the 2-mode Gaussian mixture model. As θ gets larger the primary trajectory exhibits a slower speed of sound, while the phantom trajectory remains nearer the native speed, causing a separation between the two trajectories. Near $\theta = 25^{\circ}$ the trajectories have separated enough to noticeably increase the diffusion rate, but are still not individually distinguishable. Beyond $\theta = 25^{\circ}$ the two trajectories begin to be distinguishable and thus diffusion rate begins to fall as $P_1(j,t)$ becomes bimodal. By $\theta = 55^{\circ}$ the two trajectories are completely distinguishable and the primary trajectory exhibits near zero diffusion.





4

Iteration



Figure 7.6 Example linear fits for the extraction of transport properties of rightward propagation.



 $\Delta_{P_i}^{(1)}$

2 3 4



Iteration



Figure 7.7 Example linear fits for the extraction of transport properties of leftward propagation.



Figure 7.8 Transport properties for rule 6 with $V = HP(\theta)$ under the SWP, BLK and ALT update modes. The results for rightward propagation are in column 1 and leftward propagation in column 2. Error bars show the standard uncertainties associated with slope of each fit.

CHAPTER 8 DISCUSSION AND OUTLOOK

We have defined, simulated, and explored a family of quantum elementary cellular automata (QECA). We will take this chapter to recapitulate our results, highlighting when they bear signatures of complexity. We will conclude with suggestions for future work on quantum cellular automata as complexity generating systems.

8.1 Are quantum elementary cellular automata complex?

We argue that QECA indeed exhibit elements of complexity, though certainly not all QECA may be considered complex. Specifically, we find our QECA to be complex along three of the axes of complexity: diversity, in the types of quantum states available to QECA as compared to a few typical quantum states; persistent dynamical macrostates, in the form of highly structured entanglement dynamics and emergence; and dynamic connectivity, as quantified by complex network measures computed on quantum mutual information adjacency matrices and their associated Fourier transforms.

In chapter 4 we found that well-characterized states from quantum information theory, such as the W and GHZ states as well as the localized singlet, singlet array, and random states, tend to be at extreme values of the network quantities known as network density, clustering coefficient, and disparity. This is contrasted with the average value of these quantities found at long times in QECA dynamics, which cover much more area when plotted with network measures as mutually orthogonal axes. We have shown that, while often related, the network measures offer a unique characterization of the structure of correlations in QECA dynamics, as quantified by a principal component analysis. For example, we observe a linear trend relating clustering coefficient and network density, which makes sense because dense networks are naturally more transitive. However, a principal component analysis reveals three principal components, one of which was dominated by network density, another by clustering coefficient, and the third by disparity.

Further, we have shown that the average values of these measures, with the addition of average local von Neumann entropy, tend to form clusters of simulations with like rule numbers. Meanwhile, altering the initial condition, phase gate angle, and lattice size tend to spread these clusters. For example, increasing system size from 11 to 20 can be seen to decrease disparity by a factor of one-tenth, which can be deduced by comparing panel (f) of Figure 4.7 and Figure 4.8.

While it is true that our QECA exhibit diverse average values of network quantities, there is a higher density of simulations which are still at the extreme values of the measures. Thus, some QECA exhibit clear diversity in correlation structure, but the majority of simulations result in states similar to the well-characterized and random quantum states. We also find an equally high density of simulations which saturate the von Neumann entropy, meaning there is a high degree of entanglement in these simulations. In the three-dimensional histograms presented in Section 4.3, the density of simulations that saturate the network measures and von Neumann entropy is approximately a factor of 10 larger than that of simulations with intermediate values. Such maximal entropy should not be regarded as complex because the system is characterized as maximally mixed, meaning each basis vector of the Hilbert space is equally represented in the state's density matrix. Similarly, maximal values of network quantities ought to not be regarded as signalling complexity because such saturation would mean network structure lacks the intricacies which typically characterize connectivity in complex systems. That is, a fully clustered or completely disparate network are efficiently described by a single scalar, the clustering coefficient or disparity, while a complex system like a metabolic network contains smaller clusters connected by, a strong disparate backbone.

Chapter 5 was devoted to examining QECA dynamics in the frequency domain. In particular, we quantified complexity dynamics in terms of the significant spectral features found in the power spectra of network quantities. The significance of a peak was determined using a 95% confidence red noise spectrum. Simulations for which the red noise hypothesis could not be rejected, like rule 14, were found to have a more intricate two dimension spectrum, or dispersion, when computed from the spacetime grid of expectation values $\langle \sigma_j^z \rangle$. Under the same analysis, rule 1 was found to show a dispersion relation with features like a phase dependent spatial period-doubled band structure. The period-doubled band structure is remansecent of the dispersion relation for a Bose-Einstein condensate in a periodic optical lattice.

Then, in chapter 6 we implemented the iteration-wise deviation for the bond entropy on a few specific simulations. The mean of this measure over all cuts and a segment of τ iterations quantifies the entanglement generation in those iterations. Plotting this result for adjacent segments of τ iterations illustrates a simulation's approach to equilibrium. Using this technique, we identified rule 6 as exhibiting uniquely robust persistent dynamical macrostates in the form of many body entanglement. By robust we mean relatively insensitive to changes in phase gate angle. By unique we mean that all other rules tend to show faster equilibration of entanglement as phase gate is increased.

Inspired by the entanglement dynamics observed for rule 6, we spent Chapter 7 making a detailed analysis of this rule's speed of sound and diffusion rate. Together, these transport properties characterize how the information of an initial localized defect is transferred during the first few iterations of rule 6 simulations. We found emergent, phase-gate-angle dependent transport properties, as compared to the classical version of rule 6 which used $V = \sigma_j^x$. Using a two-mode Gaussian mixture model, we were able to identify a second phantom trajectory emerging from a single localized initial condition for a phase gate angle greater than 25°. The phantom trajectory was insensitive to phase gate angle and showed high diffusion rate and speed of sound.

The broad analysis, frequency space, approach to equilibrium, and transport property analyses have lead us to conclude that our QECA exhibit complexity along three axes: diversity, persistent dynamical macrostates, and connectivity. We have found that only a limited number of simulations exhibited features which we deem complex based on these axes of complexity, but those that do, do so obviously. In particular, we found rule 6 is unique in its ability to generate complex phenomenon across more than one axis of complexity. It is possible that there are complex phenomenon in more QECA rules which were not observed in our studies. This prospect brings us to a discussion for further studies of QECA beyond what has been presented in this thesis.

8.2 Suggestions for future work

Our family of QECA models was inspired by the simplest possible classical cellular automata with nearest neighbor interactions and a local state space of two bits. As we saw in Chapter 7, introducing a quantum mechanical update operator substantially altered an otherwise well-characterized classical cellular automata. It is likely that adapting our model to include next nearest neighbor interactions – or even long-range interactions as one finds in ultracold Rydberg gas optical lattice-based quantum simulators [81, 82, 83] – will allow us to find even more complexity generating quantum cellular automata. One could also consider a larger local state space (i.e., replacing qubits with so-called qudits). However, both of these options will dramatically increase the number of rules one could simulate. For example, the number of reversible quantum cellular automata with a neighborhood of five sites, and a two dimensional local state space is given by $2^{2^4} \approx 6.55 \times 10^4$. Using techniques presented in this thesis, like the iteration-wise deviation of bond entropy, one could automatically search this large rule set for persistent dynamical macrostates. With three orders of magnitude more rules than considered here, it is likely that one would find many more complexity generating quantum cellular automata. One could then address the relative density of complex rules to non complex rules for an increasing neighborhood size (or local dimension) using genetic algorithms or other machine learning tools. Doing so provides an opportunity for yet another axis of complexity, selection principles, to enter the discussion.

Additionally, one could consider the introduction of randomness to the simulations. Randomness is key in simulating certain complex dynamics like protein folding which, without randomness, can converge to configurations which are only at a local energy minimum. The randomness in these simulations allows configurations to overcome local minimum barriers in search of a global energy minimum, completely changing the outcome of the simulation. In the case of quantum cellular automata, one could consider the introduction of quantum or classical noise to our simulations in a number of ways. One option is to introduce inhomogeneous rules which, based on the outcome of a random number generator, applies a different quantum cellular automata rule to a given site. Alternately one could consider introducing randomness into the measurement process rather than the time evolution process. This could be done by, again based on the outcome of a random number generator, adding a maximally mixed component to the single site reduced density matrices used for measuring local observables. We predict the introduction of randomness could make otherwise bland rules exhibit complex phenomenon. Because the theory of noise in quantum systems is quite subtle, we refer the interested reader to [84].

Furthermore, those QECA which display fast growth of bond entropy, like rules 5, 7, and 11, for example, would not gain substantial speed up from an approximate time evolution scheme like matrix product states. While matrix product state methods are useful for simulating much larger systems than we are able to with our exact method, they suffer from insurmountable inefficiencies when simulating highly entangled dynamics. This means that an analysis of many of the QECA defined in this thesis for much larger systems is impossible without the realization of a quantum computer, where an exponentially large Hilbert space becomes a resource rather than a nuisance [85, 42]. With a quantum computer comes the ability to simulate many orders of magnitude of neighborhood size; one could then investigate multiscale hierarchies in QECA dynamics.

The possibilities offered by quantum cellular automata are very large indeed, perhaps even astronomically large, yet another axis of complexity one might explore in the future. This thesis was an analysis of the complex phenomenon available to the simplest possible quantum cellular automata models, quantum elementary cellular automata. With future studies of quantum cellular automata as complexity generating systems, it is possible we could begin to form underlying principles of complexity generation in quantum systems. We could then leverage such complexity principles to analyze and develop complex systems of technological interest.

REFERENCES CITED

- R. E. S. J. Hartmanis, On the Computational Complexity of Algorithms. Transactions of the American Mathematical Society 117, 285 (1965).
- [2] C. S. Wallace and D. L. Dowe, Minimum Message Length and Kolmogorov Complexity. The Computer Journal 42, 270 (1999).
- [3] K. Kaneko, in Artificial Life (MIT Press, Cambridge, MA, USA, 1993), Chap. 8, pp. 163–177.
- [4] N. F. Johnson, Simply complexity : a clear guide to complexity theory (Oneworld, Oxford, 2010).
- [5] L. Tesfatsion, Agent-based computational economics: Growing economies from the bottom up. Artificial life 8, 55 (2002).
- [6] H. Ohtsuki, C. Hauert, E. Lieberman, and M. Nowak, A simple rule for the evolution of cooperation on graphs and social networks. Nature **441**, 502 (2006).
- [7] D. Stein and C. Newman, Spin Glasses and Complexity, Primers in Complex Systems (Princeton University Press, ADDRESS, 2013).
- [8] J. Sommeria, S. D. Meyers, and H. L. Swinney, Laboratory simulation of Jupiter's Great Red Spot. Nature 331, 689 (1988).
- [9] P. S. Marcus, Numerical Simulation of Jupiter's Great Red Spot. Nature 331, 693 (1988).
- [10] C. Taylor, The Atomists, Leucippus and Democritus: Fragments: a Text and Translation with a Commentary (University of Toronto Press, Toronto, 1999).
- [11] S. Wolfram, Universality and complexity in cellular automata. Physica D: Nonlinear Phenomena 10, 1 (1984).
- [12] S. Wolfram, Cellular automata as models of complexity. Nature **311**, 419 (1984).

- [13] The National Academies Keck Futures Initiative: Complex Systems: Task Group Summaries (The National Academies Press, Washington, D.C., 2008).
- [14] E. Bullmore and O. Sporns, Complex brain networks: graph theoretical analysis of structural and functional systems. Neuroscience 10, 186 (2009).
- [15] T. Matsuyama and M. Matsushita, Fractal Morphogenesis by a Bacterial Cell Population. Critical Reviews in Microbiology 19, 117 (1993).
- [16] P. W. Anderson, Basic Notions of Condensed Matter Physics (Addison-Wesley, New York, 1984).
- [17] T. Byrnes, N. Y. Kim, and Y. Yamamoto, Exciton-polariton condensates. Nature Physics 10, 803 (2014).
- [18] M. C. Gonzalez, C. A. Hidalgo, and A.-L. Barabasi, Understanding individual human mobility patterns. Nature 453, 779 (2008).
- [19] G. West, J. Brown, and B. Enquist, The fourth dimension of life: Fractal geometry and allometric scaling of organisms. Science 284, 1677 (1999).
- [20] P. Grassberger and I. Procaccia, Characterization of Strange Attractors. Physical Review Letters 50, 346 (1983).
- [21] J. M. Carlson and J. Doyle, Complexity and Robustness. Proceedings of the National Academy of Sciences 99, 2538 (2002).
- [22] S. P. Stromberg and J. Carlson, Robustness and Fragility in Immunosenescence. Public Library of Science Computational Biology 2, 1475 (2006).
- [23] J. B. S. Haldane, On Being the Right Size. Harper's Magazine (1926).
- [24] S. Braun *et al.*, Emergence of coherence and the dynamics of quantum phase transitions. Proceedings of the National Academy of Sciences **112**, 3641 (2014).
- [25] A. L. Goodman *et al.*, Identifying Genetic Determinants Needed to Establish a Human Gut Symbiont in Its Habitat. Cell host & Microbe 6, 279 (2009).
- [26] V. Amendola and M. Meneghetti, Self-healing at the nanoscale. Nanoscale 1, 74 (2009).

- [27] G. Hinton *et al.*, Deep neural networks for acoustic modeling in speech recognition: The shared views of four research groups. Signal Processing Magazine, IEEE **29**, 82 (2012).
- [28] M. E. J. Newman, The Structure and Function of Complex Networks. Society of Industrial and Appplied Mathematics Review 45, 167 (2003).
- [29] M. Newman, Networks: An Introduction (Oxford University Press, Inc., New York, NY, USA, 2010).
- [30] J. A. Dunne, R. J. Williams, and N. D. Martinez, Network structure and biodiversity loss in food webs: robustness increases with connectance. Ecology Letters 5, 558 (2002).
- [31] O. Güell, F. Sagués, and M. Ángeles Serrano, Detecting the Escherichia coli metabolic backbone. ArXiv e-prints (2014).
- [32] M. Planck, On the Law of Distribution of Energy in the Normal Spectrum. Annalen der Physik 4, 553 (1901).
- [33] C. Johnson, Mathematical Physics of BlackBody Radiation. Icarus iDucation. Skolan för datavetenskap och kommunikation, Kungliga Tekniska Högskolan, Stockholm (2012).
- [34] A. Einstein, On a heuristic viewpoint concerning the production and transformation of light. Annalen der Physik 17, 132 (1905).
- [35] K. Riley, M. Hobson, and S. Bence, *Mathematical Methods for Physics and Engineering:* A Comprehensive Guide (Cambridge University Press, Cambridge, 2006).
- [36] K. Gottfried and T. Yan, Quantum Mechanics: Fundamentals, Graduate Texts in Contemporary Physics (Springer, New York, 2003).
- [37] C. H. Bennett and G. Brassard, in Proceedings of IEEE International Conference on Computers, Systems, and Signal Processing (IEEE, India, 1984), p. 175.
- [38] L. K. Grover, in ANNUAL ACM SYMPOSIUM ON THEORY OF COMPUTING (ACM, ADDRESS, 1996), pp. 212–219.
- [39] W. Pauli, The Connection Between Spin and Statistics. Physical Review 58, 716 (1940).

- [40] P. G. Kevrekidis, D. J. Frantzeskakis, and R. Carretero-González, Emergent nonlinear phenomena in Bose-Einstein condensates: theory and experiment (Springer Science & Business Media, New York, 2007), Vol. 45.
- [41] D. Griffiths, Introduction to Quantum Mechanics, Pearson international edition (Pearson Prentice Hall, New Jersey, 2005).
- [42] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information: 10th Anniversary Edition, 10th ed. (Cambridge University Press, New York, NY, USA, 2011).
- [43] M. M. Wolf, F. Verstraete, M. B. Hastings, and J. I. Cirac, Area Laws in Quantum Systems: Mutual Information and Correlations. Physical Review Letters 100, 070502 (2008).
- [44] D. L. Vargas and L. D. Carr, Detecting Quantum Phase Transitions via Mutual Information Complex Networks. ArXiv e-prints (2015).
- [45] S. Wolfram, A New Kind of Science (Wolfram Media, Champaign, 2002), p. 1197.
- [46] D. Gage, E. Laub, and B. McGarry, in *Proceedings of the Midwest NKS Conference* (Springer, New York, NY, 2005).
- [47] M. Cook, Universality in elementary cellular automata. Complex systems 15, 1 (2004).
- [48] R. Feynman, Simulating physics with computers. International Journal of Theoretical Physics 21, 467 (1982).
- [49] G. Grossing and A. Zeilinger, Quantum cellular automata. Complex Systems 2, 197 (1988).
- [50] J. Kempe, Quantum random walks: an introductory overview. Contemporary Physics 44, 307 (2003).
- [51] J. Watrous, in In 36th Annual Symposium on Foundations of Computer Science (Society Press, Milwaukee, 1995), pp. 528–537.
- [52] W. van Dam, Master's thesis, Computer Science Nijmegen, 1996.

- [53] C. Durr, H. LeThanh, and M. Santha, A decision procedure for well-formed linear quantum cellular automata. Proceedings of the 13th Annual Symposium on Theoretical Aspects of Computer Science (1999).
- [54] P. Arrighi, V. Nesme, and R. Werner, Unitarity plus causality implies localizability. Journal of Computer and System Sciences (2009).
- [55] R. Raussendorf, Quantum cellular automaton for universal quantum computation. Physical Review A 72, 022301 (2005).
- [56] D. J. Shepherd, T. Franz, and R. F. Werner, Universally Programmable Quantum Cellular Automaton. Physical Review Letters 97, 020502 (2006).
- [57] B. Schumacher and R. F. Werner, Reversible quantum cellular automata. eprint arXiv:quant-ph/0405174 (2004).
- [58] C. A. Pérez-Delgado and D. Cheung, Local unitary quantum cellular automata. 76, 032320 (2007).
- [59] D. A. Meyer, From quantum cellular automata to quantum lattice gases. Journal of Statistical Physics 85, 551 (1996).
- [60] G. K. Brennen and J. E. Williams, Entanglement dynamics in one-dimensional quantum cellular automata. 68, 042311 (2003).
- [61] D. Bleh, T. Calarco, and S. Montangero, Quantum Game of Life. Europhysics Letters (2010).
- [62] G. L. Snider *et al.*, Quantum-dot cellular automata. Journal of Vacuum Science & Technology A 17, 1394 (1999).
- [63] P. TOUGAW and C. LENT, Logical devices implemented using quantum cellular automata. Journal of Applied Physics 75, 1818 (1994).
- [64] R. Cowburn and M. Welland, Room temperature magnetic quantum cellular automata. Scienced 287, 1466 (2000).
- [65] A. Imre *et al.*, Majority logic gate for magnetic quantum-dot cellular automata. Science 311, 205 (2006).

- [66] D. Bera, L. Qian, T.-K. Tseng, and P. H. Holloway, Quantum Dots and Their Multimodal Applications: A Review. Materials 3, 2260 (2010).
- [67] W. K. Wootters and W. H. Zurek, A single quantum cannot be cloned. Nature 299, 802 (1982).
- [68] Quantum cellular automata based on elementary cellular automata, http://www.github.com/lhillber/qca, accessed: 2016-04-15.
- [69] A. Collette, Python and HDF5 (Oreilly & Associates Incorporated, Sebatpol, 2013).
- [70] L. Dalcn, R. Paz, and M. Storti, MPI for Python. Journal of Parallel and Distributed Computing 65, 1108 (2005).
- [71] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states. Annals of Physics **326**, 96 (2011).
- [72] M. L. Wall and L. D. Carr, Out of equilibrium dynamics with matrix product states. New Journal of Physics 14, 125015 (2012).
- [73] M. Suzuki, Convergence of general decompositions of exponential operators. Communications in Mathematical Physics 163, 491 (1994).
- [74] R. Armstrong et al., in High Performance Distributed Computing, 1999. Proceedings. The Eighth International Symposium on High Performance Distributed Computing (IEEE, New York, NY, 1999), pp. 115–124.
- [75] T. M. Forum, MPI: A Message Passing Interface, 1993.
- [76] T. Shanley, x86 Instruction Set Architecture. (2010).
- [77] W. M. Hartmann, Signals, sound, and sensation, Modern acoustics and signal processing, corrected 5th printing ed. (American Institute of Physics, Woodbury, NY, 2005).
- [78] W. Navidi, Statistics for Engineers and Scientists, McGraw-Hill Higher education (McGraw-Hill, New Yoirk, NY, 2010).
- [79] M. Machholm, C. Pethick, and H. Smith, Band structure, elementary excitations, and stability of a Bose-Einstein condensate in a periodic potential. Physical Review A 67, 053613 (2003).

- [80] B. Seaman, L. Carr, and M. Holland, Period doubling, two-color lattices, and the growth of swallowtails in Bose-Einstein condensates. Physical Review A **72**, 033602 (2005).
- [81] R. Loew *et al.*, An experimental and theoretical guide to strongly interacting Rydberg gases. J. Phys. B. - At. Mol. Opt. Phys. 45, (2012).
- [82] J. Schachenmayer, I. Lesanovsky, A. Micheli, and A. J. Daley, Dynamical crystal creation with polar molecules or Rydberg atoms in optical lattices. New Journal of Physics 12, 103044 (2010).
- [83] L. D. Carr, D. Demille, R. V. Krems, and J. Ye, Cold and Ultracold Molecules: Science, Technology, and Applications. New Journal of Physics 11, 055049 (2009).
- [84] A. A. Clerk *et al.*, Introduction to quantum noise, measurement, and amplification. Reviews of Modern Physics 82, 1155 (2010).
- [85] D. P. Divincenzo, The Physical Implementation of Quantum Computation. Fortschritte der Physik 48, 771 (2000).