UNIVERSITY OF WATERLOO

FACULTY OF SCIENCE

Quantum Cellular Automata and Black Hole Evaporation

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Program and Term
Mathematical Physics 2A

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Brian McNamara, Department Chair
Physics and Astronomy,
Faculty of Science,
University of Waterloo
200 University Ave West
Waterloo, ON, N2L 3G1

Dear Professor McNamara,

This report, titled "Quantum Cellular Automata and Black Hole Evaporation", was prepared after my 2A term in Mathematical Physics, and was my first work term report for Wolfram Research. The purpose of this report is to attempt to recreate the Page curve for Hawking radiation using quantum cellular automata.

Wolfram research is a company that makes computational technology, including WolframAlpha and Mathematica. My job at this company was to add functionality to their upcoming Quantum Computing / Quantum Mechanics framework. I have used this framework to conduct my research. I am in the Algorithms and Research department, and my supervisor is Jose Martin-Garcia.

I would like to thank my manager, Jonathan Gorard, for providing inspiration, encouragement, and direction to write this report, and constantly answering any questions I had. I would also like to thank the PD11 TAs for their support. I have read over and formatted this report. This report was written entirely by me and has not received any previous academic credit at this or any other institution.

Sincerely,
Ruhi Shah
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1 Summary

A new formalism for Quantum Cellular Automata (QCA) and a weighted von Neumann entropy is used to attempt to reproduce the Page curve from Hawking radiation. The QCA is used to model a black hole and its radiation, and the weighted von Neumann entropy is used to measure the entanglement entropy of the black hole. First, a new formalism for QCAs is introduced, one that evolves mixed states. An event horizon is added to the QCA to represent a more complete picture of space time. A new weighted version of von Neumann entropy is also introduced. The two are then subsequently used to attempt to recreate the Page curve. Several aspects of the Page curve are recovered for certain values of weighting factors in the weighted von Neumann entropy, including initial purity, reaching a maximum value, and returning back to purity.

2 Introduction

When Hawking first discovered the fact that black holes emit particles (now known as Hawking radiation), a great paradox emerged (Hawking, 1975). The existence of Hawking radiation implied the evaporation of black holes, and everything that ever fell into them (Hawking, 1975). According to the laws of quantum mechanics, this is impossible, since information must always be conserved. This meant that the evolution of a black hole must be unitary, or reversible. Given any state of the black hole and its radiation at one point in time, we should be able to determine the state at any other point in time (Barbón, 2009).

In order to solve this problem, Hawking suggested that there must be information contained in the Hawking radiation released by a black hole, quantified through the entanglement entropy of the radiation (Barbón, 2009). The von Neumann entropy is a way to measure the entanglement entropy of a system (Neumann et al., 2018). Just as the classical Shannon entropy describes the uncertainty of the probability distribution of a system, the von Neumann entropy describes the uncertainty in the probability distribution of a quantum state (Nielsen and Chuang, 2016).

Consider the creation of a black hole, everything about the initial state is known, the state is pure, and so in the beginning, the black hole has an entanglement entropy of zero. As the black hole evaporates, the particles radiating out will be entangled with the particles inside, and the entanglement entropy of the entire system will increase. However, according to the laws of quantum mechanics, the entire black hole system must return to a pure state (once all the radiation has escaped, and the black hole has evaporated). Assuming that the black hole does evolve unitarily, we would expect it to begin with an entanglement entropy of 0, and then increase in entropy, and then return back to 0 (Barbón, 2009). This evolution is known as the Page curve for Hawking radiation, and it describes the entanglement entropy of the black hole and its radiation over time (Page, 1993).

The goal of this report is to attempt to recreate the Page curve for Hawking radiation using a suitable toy model for black holes. The Page curve has been recovered before from semi-classical geometry (Almheiri et al., 2019). However, this report will attempt to do the same using Quantum Cellular Automata (QCAs). Often when dealing with unitary evolution of quantum systems, it helps to use QCAs (Arrighi, 2019). In the context of black hole thermodynamics, this has already been done in a previous publication (Shah and Gorard, 2019).

Other than the interesting computational model that will come out of this research, the report also contributes to the upcoming Wolfram Physics project. Currently, there are certain computational limitations that limit the simulation and study of quantum entanglement. The QCA model in this paper can provide a way to simulate quantum entanglement, in a similar context to that of the Wolfram Physics project, while still being computationally feasible. By recreating the Page curve, this model will prove its validity in the context of the Wolfram Physics project.

In this report, a formalism to investigate these black hole systems is described. It consists of a QCA formalism that starts with an initial state of $|\psi_0\rangle$, and evolves the state with a unitary matrix U. In order to investigate the information contained in the black hole radiation, a modified version of the von Neumann entropy of a toy black hole is introduced, properties of which will be proven subsequently. The results found when using this QCA formalism and the new entanglement entropy will then be analysed for interesting features and connections to the Page curve.

3 Formalism

3.1 QCA Formalism

A QCA is a quantized version of Cellular Automata (CA), where instead of evolving an arrangement of bits using a universal evolution rule, an arrangement of *qubits* is evolved using a *unitary* universal evolution rule (Arrighi, 2019). In this paper, the evaporation of a black hole is modelled using a QCA. All the code used to simulate the QCA was written using Mathematica. All figures in this report are primary sources. They were either made using Google Drawings, or generated from the code used to simulate the QCA. The code and algorithm itself was an extension of the function QuantumTensorAutomaton that is in the Wolfram function repository (Shah and Gorard, 2019).

The formalism for the QCA greatly resembles the one in earlier work. First the density matrix of a pure state is taken. Then, an arity-3 unitary operator is applied on to sets of three qubits.

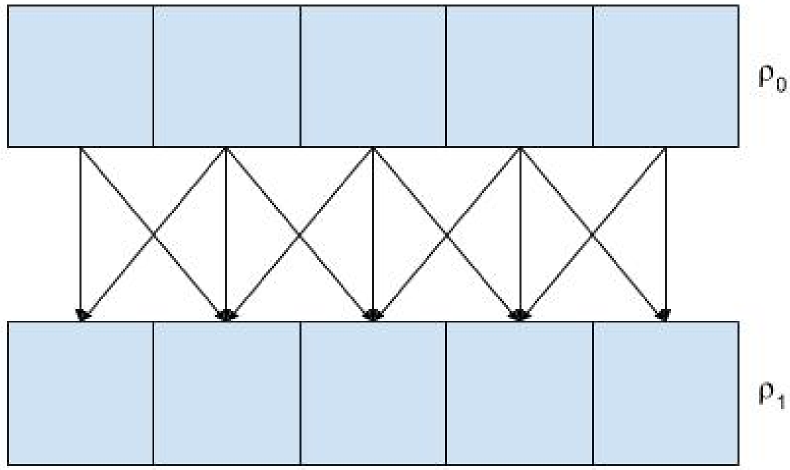

Figure 1: Visual representation of the evolution of a QCA. The array of blue squares represents five different qubits, and the arrows show which qubits affect the evolution of a specific qubit.

The resulting states are then added together. Overall, the evolution operator is unitary, since each individual operator applied is unitary.

For an n-qubit system, and a unitary operator u that inputs three qubits and outputs three qubits, the evolution operator can be expressed as following.

$$U = \sum_{i=1}^{n} u^{(i-1,i,i+1)} \tag{1}$$

Starting with a state ρ_0, and the evolution operator U in (2), the next state ρ_1 is then:

$$\rho_1 = U \rho_0 U^{\dagger}$$

3.1.1 Periodic Boundary Conditions

The first system that was investigated used the evolution operator (1), with periodic boundary conditions. This meant that the first qubit would have the last qubit as its right neighbour. This is not a physically reasonable model. There was also no clear distinction between the outgoing radiation, and the black hole itself. Since both aspects of the system behave drastically differently, a distinction between the two is essential to have a physically reasonable model. Nevertheless, a basic model with periodic boundary conditions was still useful for investigation of certain properties.

The QCA was run for a few steps, and the resulting diagonal elements of each density matrix ρ_i were plotted. There was a phase shift that occurred for certain diagonal elements; the probability would increase, reach a maximum, and then decrease. Specifically, the probability of the qubits being in the first basis state followed certain aspects of the Page curve. Calculating the von Neumann entropy using a weighted trace would allow the first basis state to dominate, and allow the Page curve to be shown in the evolution of the entropy of the system as well.

This model was used along with the modified entropy in section 4.2.1, and the results of that investigation are presented in section 5.1.

3.1.2 Including an Event Horizon

A more elaborate version of boundary conditions makes the model more physically realizable. First, an event horizon was added. Since the QCA is one-dimensional, all the information about the black hole is encoded in the qubit that is at the event horizon (Barbón, 2009). Again, this is not ideal, but due to computational limitations, a two or three dimensional QCA was not feasible. This event horizon will separate the inside and outside of the black hole (the outgoing radiation and interior), and overtime, the event horizon will move as the black hole evaporates. When the event horizon reaches the end of the array of qubits, the evaporation of the black hole is complete (Figure 2).

The exact workings of the event horizon had to do with quantifying the neighbours of each individual qubit. It was assumed that a qubit inside the black hole has no access to its neighbours. So, for each qubit inside the black hole (or to the right of the event horizon), the neighbours are taken to be the one qubit density matrix: $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$. This was done since a state inside the black hole may be thought of as being maximally mixed to other states, although there is no evidence or support for this claim. For qubits at the edge of an array (either a first or last qubit), the missing neighbouring qubit was taken to be the one qubit density matrix: $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$. This was done since the neighbour of a state on the outside may be a fixed environment of sorts, one that was entirely deterministic,

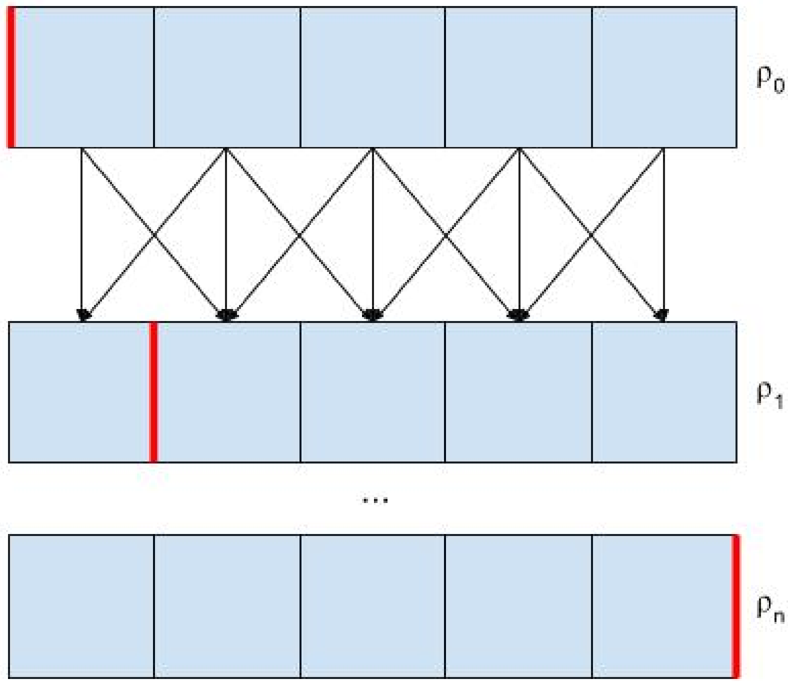

Figure 2: Visual representation of the evolution of a QCA with an event horizon. The array of blue squares represents five different qubits, the arrows show which qubits affect the evolution of a specific qubit, and the red line represents the event horizon. The qubits to the left are the Hawking radiation, the qubits to the right are in the black hole. Each step of the evolution moves the horizon one step to the right. ρ_0 and ρ_n should both be pure states.

although again, there is no evidence or support for this claim.

It is important to note that in this model, at each time step, one qubit worth of information is evaporated. However, this is not necessarily the case in black hole evaporation. This model was used along with the modified entropy in section 4.2.2, to give more physically reasonable results than the basic model, as seen in section 5.2.

3.2 Entanglement Entropy

The entanglement entropy of the entire state, both the black hole and its radiation, is measured. If the QCA is able to reasonably model a black hole, the entropy of the QCA should follow a Page curve when it is evolved through time (Barbón, 2009). A modified definition of von Neumann entropy was used to investigate the QCA.

In the QCA, a pure quantum state is evolved into a mixed state, both of which can be described using a density matrix, ρ. Each density matrix has a spectral decomposition (Nielsen and Chuang, 2016).

$$\rho = \sum_i \lambda_i \langle \psi_i || \psi_i \rangle$$

Since each of the λ_i are real, the classical von Neumann entropy can be defined based on them (Nielsen and Chuang, 2016).

$$V(\rho) = \sum_i -\lambda_i \ln \lambda_i \tag{2}$$

This is the method of calculating the von Neumann entropy that is used throughout this paper, since each density matrix has a spectral decomposition (which is generally true). Although, for different methods of calculation, the ultimate numerical result is the same (Nielsen and Chuang, 2016).

3.2.1 Weighted von Neumann Entropy

The weighted version of the von Neumann entropy is:

$$V_w(\rho) = \sum_i -\frac{1}{i} \lambda_i \ln \lambda_i \tag{3}$$

This version of the von Neumann entropy has several of the same properties as the original von Neumann entropy (1), including subaddivity, concavity, and certain others.

3.2.2 Modifying the Scaling factor

A more physically realizable version of this definition involves treating the "weighting" term in (3) as loosely equivalent to a gamma factor in special relativity. This places the QCA in some form of a

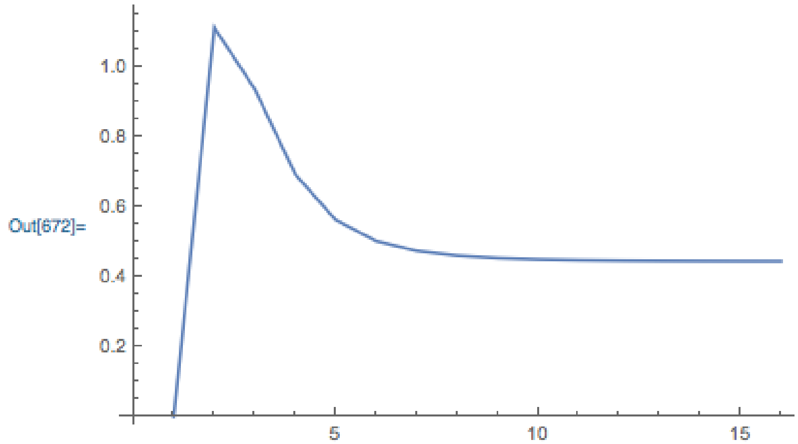

Figure 3: Evolution of a basic QCA model. This is the evolution of a random pure initial state and a random unitary evolution operator for 15 time steps.

spacetime, where motion away from the black hole may have effects on the entropy of the system. For an n-qubit system, the new dialated entropy is:

$$V_w(\rho) = \sum_{i=1}^{2^n} -(\frac{1}{i} - \frac{1}{n})\lambda_i \ln \lambda_i \tag{4}$$

Although, i does not specify the i^{th} qubit, this factor, for reasons unknown, provides interesting results. It also follows the same properties as (1). This is shown in section 5.2.

4 Investigating the Resulting Page Curve

4.1 Basic Formalism

For the basic formalism, using the evolution operator in (1), and the weighted entropy in (3), a random initial state and a random unitary evolution operator creates a curve like in Figure 3.

Clearly, although there is a phase shift, this is not the Page curve. The Page curve requires an entropy maximum at approximately half the total evolution time and a final entropy of zero (Page, 2013), neither of which show up in this result. However, this simple model can still be analysed.

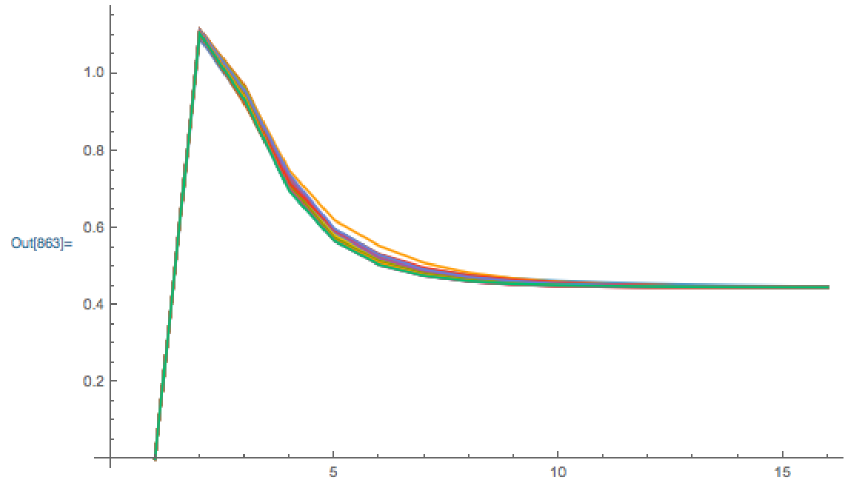

Figure 4: Evolution of a basic QCA model for a fixed operator and 30 different random pure initial conditions. Each different initial condition refers to a different coloured line.

4.1.1 Effect of Initial Conditions and Unitary Operators on the Evolution

In research done in (Shah and Gorard, 2019), analysis was done on different initial conditions, different evolution operators, and how they affected the equilibrium time of the QCA. A similar analysis was done here, on how changing initial conditions and evolution operators affects the Page time. The Page time is the time in the evolution of the black hole at which the entanglement entropy begins to decrease, or the time at which the maximum entanglement entropy occurs. For a black hole beginning with a pure state, it is expected to occur at approximately half the total evolution time (Page, 2013).

For the basic model, the Page time occurred 1 or 2 steps into the 6-step evolution, for all random unitary operators, and all random pure initial conditions tested, not half way.

From Figures 3 and 4, the shape of the curve is unaffected by the actual unitary operator, or the initial condition used. The Page time is predicted to be around half the total evolution time for an initially pure state (Page, 2013). In the case of the QCA, this time doesn't make sense, since our model evolves for an "infinite" amount of time, of which there is no half of. The Page time generally occurs when the black hole becomes Planckian (Barbón, 2009). However, due to the small number of qubits in our investigation, the black hole is already Planckian to begin with. This might be what

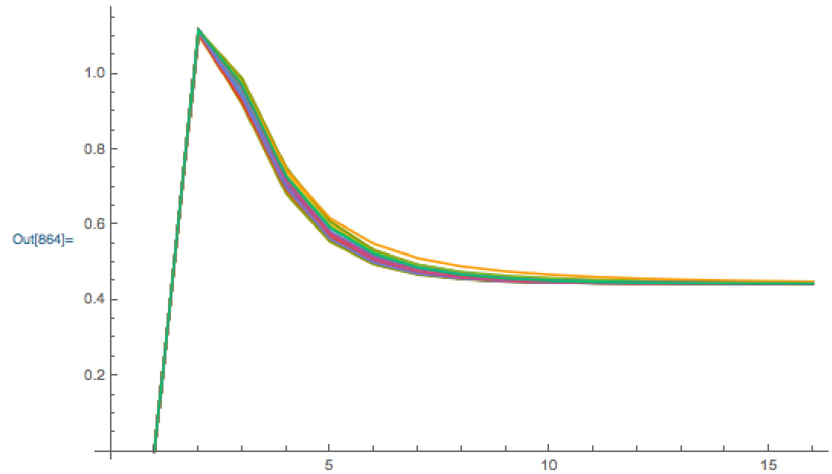

Figure 5: Evolution of a basic QCA model for a fixed initial state and 30 different random unitary operators. Each different unitary operator refers to a different coloured line.

is causing the early phase shift.

4.1.2 Effects of Increasing the Number of Qubits on the Evolution

Although changing the initial conditions, and the evolution operator leaves the curve unaffected, increasing the number of qubits brings the final equilibrium entropy closer and closer to zero (Figure 6). As the number of qubits are increased to an extremely large number (as usually is the case, when non-microscopic black holes are considered), the limit will converge to zero.

So far, inputs and outputs of the QCA have been modified. However, small modifications in the model itself might provide some insight into making a more physically realizable model. This will be done in the next section.

4.2 Physically Realizable Formalism

4.2.1 Effect of Initial Conditions and Unitary Operators on the Evolution

Following the QCA formalism in 4.1.2 and the entanglement entropy in 4.2.2, a random pure initial condition, and a random unitary operator will create an evolution shown in Figure 7. Again, changing initial conditions and changing operators does not affect the Page time of the evolution

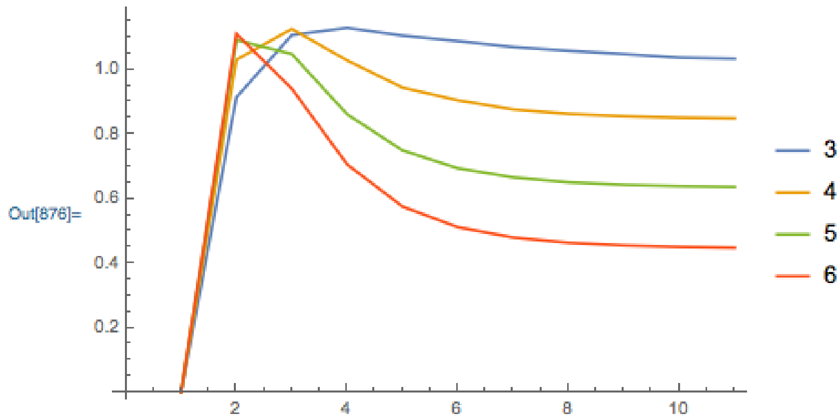

Figure 6: Evolution of a basic QCA model for different amounts of qubits. Each initial pure state is a maximally entangled qubit, and the operator is the same for all. The legend shows what colour corresponds to the what number of qubits. As you increase the number of qubits, the final entropy gets closer and closer to zero.

(Figure 8 and 9). Also, increasing the number of qubits brings the final entropy closer to zero (Figure 10). These results are the same as in section 5.1.

However, changing the unitary operator significantly affects the final entropy, sometimes making it very close to zero (which is what is required in the Page curve), and can be seen in Figure 7. Keeping the initial state to be constant, and looking at 50 different random unitary operators, the final entropy of each QCA was found. The mean of the final entropy with different operators had a standard deviation of approximately 0.06. Keeping the evolution operator constant, and looking at 50 different random initial conditions, the final entropy of each evolution was found again. The mean of the final entropy for different initial conditions had a standard deviation of approximately 0.002. The operators affect the final entropy much more than the initial conditions, and this can also be seen in Figure 8 and 9. Changing initial conditions does not significantly vary this final entropy.

4.2.2 Finding the Optimal Scaling Factor

There are certain aspects of this model that can be varied to get better results. The first thing is the scaling term in (4), there is no apparent reason why the constant $\frac{1}{n}$ may be optimal. For a system of five qubits, that constant was changed, and the resulting average final entropy value over different

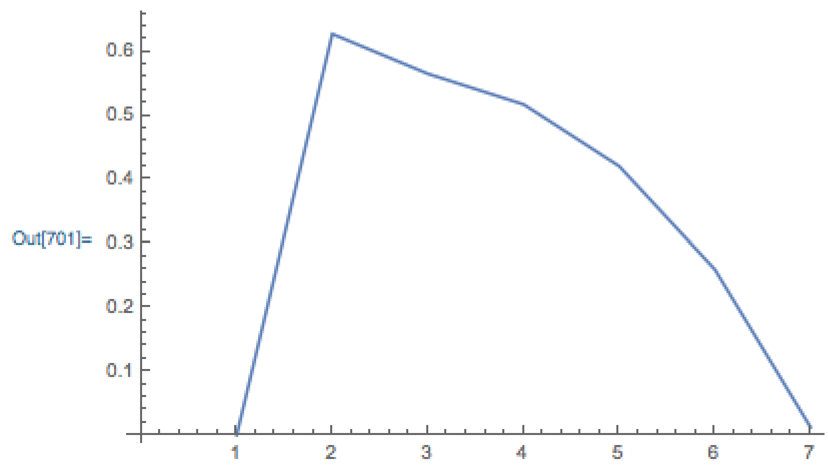

Figure 7: Evolution of a physically reasonable QCA model with a random unitary evolution operator and a random initial condition.

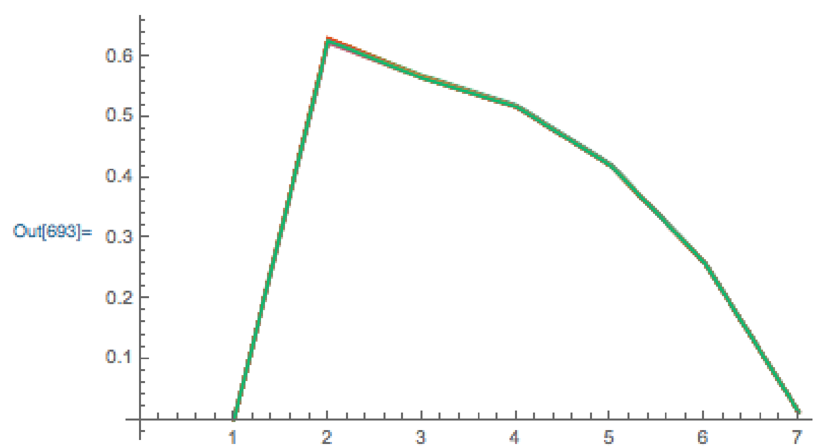

Figure 8: Evolution of a physically reasonable QCA model with a fixed operator and 30 different random pure initial conditions. Each different initial condition refers to a different coloured line.

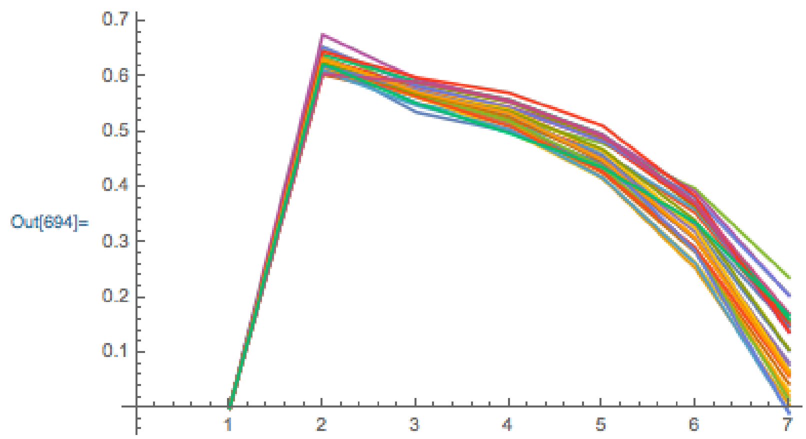

Figure 9: Evolution of a basic QCA model for a fixed initial state and 30 different random unitary operators. Each different unitary operator refers to a different coloured line.

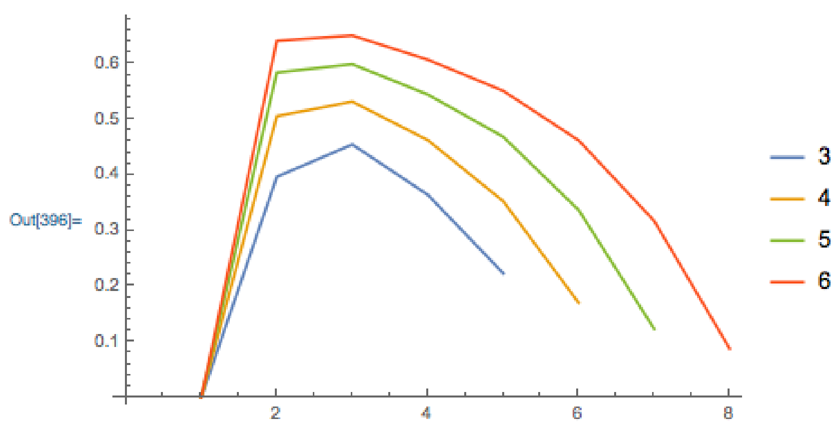

Figure 10: Evolution of a physically reasonable QCA model for different amounts of qubits. Each initial pure state is a maximally entangled qubit, and the operator is the same for all. The legend shows what colour corresponds to the what number of qubits. As you increase the number of qubits, the final entropy gets closer and closer to zero.

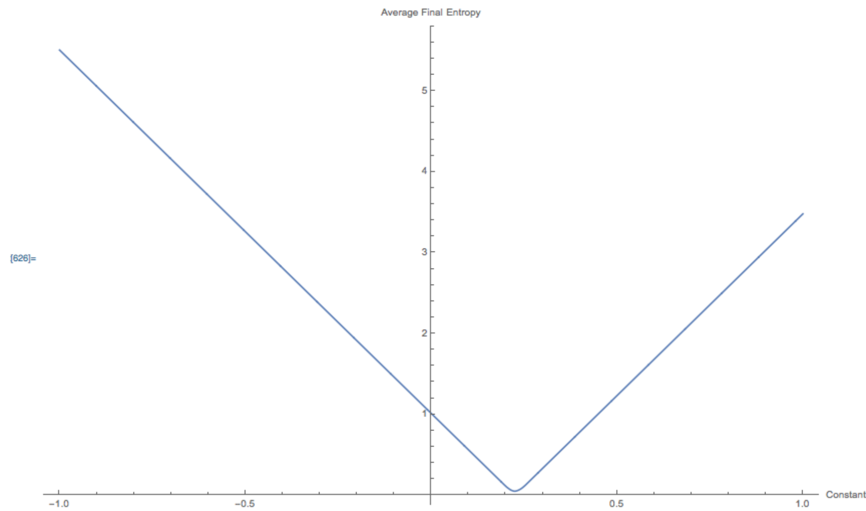

Figure 11: Finding the optimal value of the constant. Values for the $\frac{1}{n}$ term in equation 4 is varied between -1 and 1 with intervals of 0.01. For each constant term, the final entropy averaged over 50 random operators is plotted.

operators was calculated (Figure 11). The minimum final entropy turns out to be close to $\frac{1}{n}$, but not exactly that. The constant was calculated to three decimal places, and turns out to be approximately 0.225. Reasons for where this constant comes from is still unknown.

Since the optimal constant is close to $\frac{1}{n}$, it can be speculated that scaling factor in (4) is correct, and the operators greatly determine the final entropy. This would mean that certain unitary operators are "valid" evolution rules for a black hole. However, this claim is pure speculation, and needs rigorous analytical analysis to be supported.

5 Conclusion and Recommendations

The Page curve was not found. However, several aspects of it were recovered. A QCA formalism was introduced, along with a weighted version of the von Neumann entropy. This formed a basic model for black hole evaporation. The basic model presented contained a phase shift, convergence to a fixed value (though not zero). It was also found that the initial conditions do not significantly affect the Page time or the final equilibrium entropy. Neither does the unitary evolution operator. Increasing the number of qubits converges the final entropy to zero. This model does not sufficiently describe black hole evaporation, but may have interesting applications elsewhere.

Then, an updated QCA formalism was introduced with a moving event horizon. This caused the evolution to become of finite length, particularly the length of the QCA itself. Along with this, an updated version of the weighted von Neumann entropy was presented, with a constant that was varied. An optimal value for the constant was found. The physically realizable model provided better results, though still was unable to sufficiently reproduce the Page curve. In this model, the phase shift occurs three steps into the evolution. The maximum entropy increases and the final entropy decreases as we increase the number of qubits. For the optimal value of the constant in the modified entropy, the final entropy has a value that is close to zero, but still is not exactly zero.

There are several future directions for this research. Firstly, rigorous mathematical analysis can be done in order to derive more concrete results conclusions, and provide analytical support to the empirical claims. Specifically, a minimum value for the constant described in the modified entropy could be analytically derived, and compared to see if it corresponds with the empirical result. Furthermore, a better version of the modified entropy can be defined, with the weighted term corresponding to a gamma factor in special relativity. The entropy of each qubit could also depend on and be modified based on the distance from the singularity. A more speculative direction includes providing support for ER = EPR (Susskind, 2016). ER = EPR states that Einstein-Rosen bridges (wormholes) are equivalent to Einstein-Podolsky-Rosen pairs (entangled particles), stemming from the fact that if two entangled systems are collapsed into black holes, there would be an Einstein-Rosen bridge between them. The modified entropy can be applied to a toy black hole in a more relativistic model, like the one in (Almheiri et al., 2019), and if the results also give a Page curve, this can provide strong support for ER = EPR.

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