Non-completely positive dynamics as a probe of entanglement in quantum circuits

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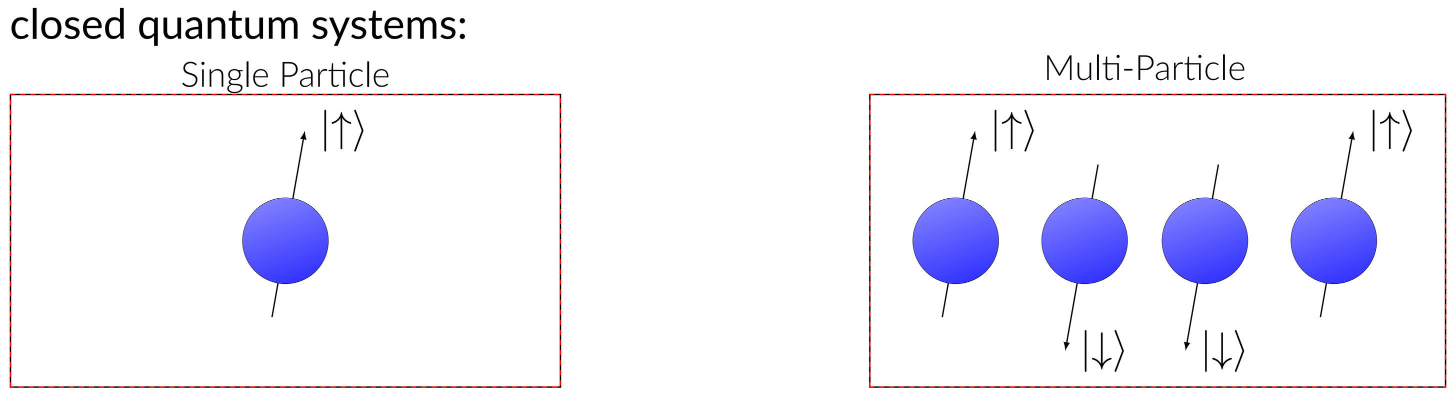
Open Quantum Systems

To describe open quantum systems, we must first review the crucial elements of **closed quantum systems:**



Single particle:
1) "Fixed" States: $|\psi\rangle = |\uparrow\rangle, |\downarrow\rangle$
2) Superposition: $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$
3) Mixed States: $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

Evolution:

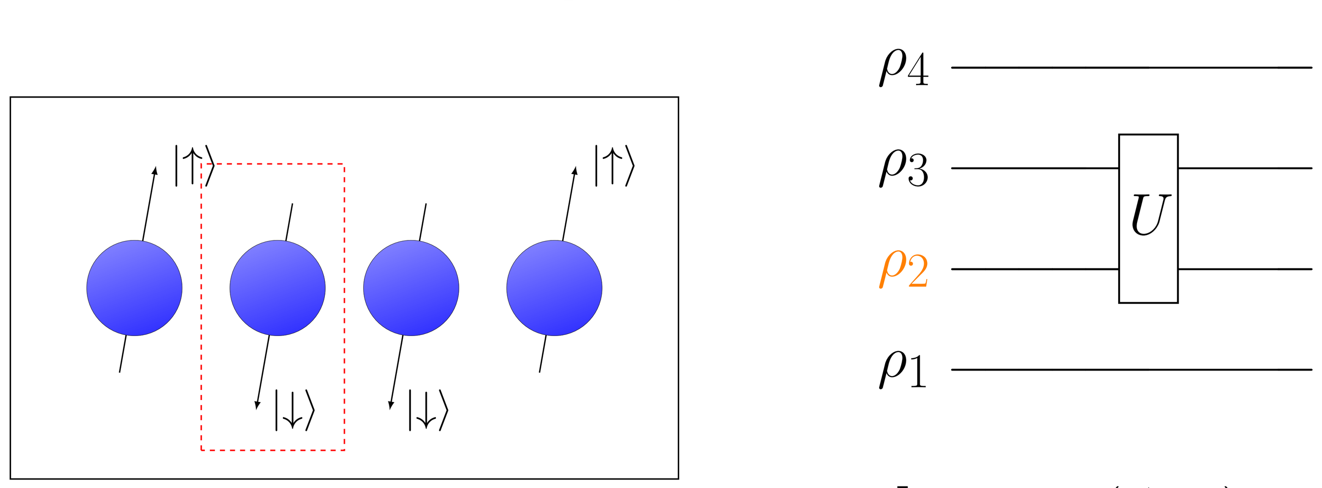
$$\hat{H}|\psi\rangle = i\hbar\frac{d}{dt}|\psi\rangle$$

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

$$\rho(t) = U(t)\rho(0)U^\dagger(t)$$

Multi-particle:
1) "Fixed" States: $|\psi\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle, |\uparrow\downarrow\uparrow\downarrow\rangle, \ldots, |ijkl\rangle$
2) Superposition & Entangled States: $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\downarrow\rangle), \ldots, \sum_{ijkl} p_{ijkl}|ijkl\rangle$
3) Mixed States: $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$

Open quantum systems are described in a similar framework, the key additions being the **partial trace** $\mathrm{Tr}_{\mathrm{env}}[\ldots]$, which is effectively an average over a subsystem's environmental correlations, and the linear **maps** Λ_i derived when considering the individual evolution of interacting subsystems.



$$\rho_S = \mathrm{Tr}_E[\rho_{SE}]$$

$$\rho_S(t) = \mathrm{Tr}_E[U(t)\rho_{SE}(0)U^\dagger(t)]$$

$$\rho_2^{(f)} = \mathrm{Tr}_{134}\left[(\mathbb{1}\otimes U\otimes \mathbb{1})\left(\bigotimes_{i=1}^{4}\rho_i^{(i)}\right)(\mathbb{1}\otimes U\otimes\mathbb{1})^\dagger\right]$$

$$\equiv \rho_2^{(f)} = \Lambda_2\rho_2^{(i)}$$

Most importantly, because maps are derived by averaging over environmental correlations, these operators are no longer required to take all valid quantum states to other valid quantum. A map that exhibits this property is **not completely positive** (NCP).

The Pauli form for single qubit states is given by

$$\rho = \frac{1}{2}\left(\mathbb{1} + \sum_i a_i\sigma_i\right) \quad (1)$$

where $i \in \{x, y, x\}$, $a_i = \mathrm{Tr}[\rho\sigma_i]$ and the condition

$$\vec{a} = \sqrt{a_x^2 + a_y^2 + a_z^2} \leq 1 \quad (2)$$

must be satisfied if ρ is to be a valid quantum state. Valid density matrices also must only have positive eigenvalues $\lambda_i \geq 0 \ \forall \ i$. This Pauli form is visually represented by the **Bloch sphere**, shown in Fig. 1.

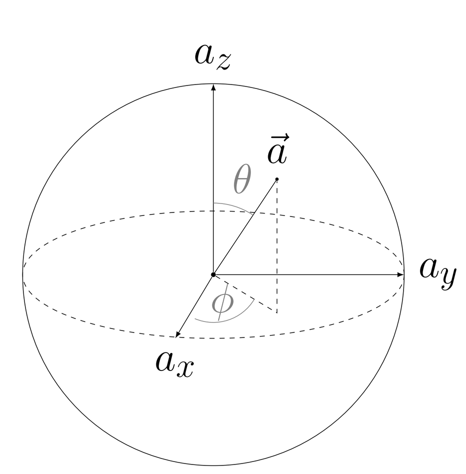


Figure 1. The Bloch sphere.

Maps on single qubit states are often visually represented by how they transform the Bloch sphere.

An example of an NCP map's action on the Bloch sphere is shown in Fig 2.

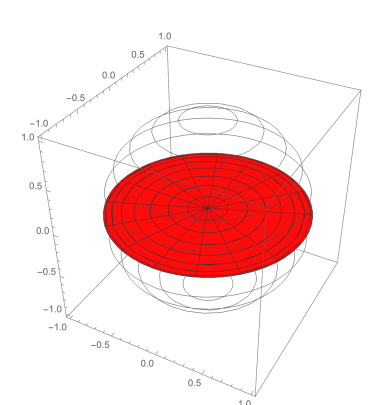


Figure 2. Action of the NCP pancake map on the Bloch sphere [1].

Another important measure is the **concurrence** between a qubit pair, which is standard a measure of bipartite entanglement, defined as

$$\mathcal{C} := \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}. \quad (3)$$

Our System & Animating the Domain of Positivity

We consider N initially uncorrelated qubits in thermal density matrices of the form $\rho_{(i)} = (1-p_i)|0\rangle\langle 0| + p_i|1\rangle\langle 1|$ Where $|0\rangle$ and $|1\rangle$ are the ground and excited state. We evolve pairs of qubits in a **brickwork circuit** using a unitary of the general form

$$\hat{U}_{2Q} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & e^{i\phi}\sin\theta & 0 \\ 0 & -e^{-i\phi}\sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (4)$$

For each qubit ρ^{AB} pair, we convert to the basis

$$\rho^{AB} = \frac{1}{4}\left(\mathbb{1}_{AB} + \sum_i A_i(\sigma_i\otimes\mathbb{1}_B) + \sum_i B_i(\mathbb{1}_A\otimes\sigma_i) + \sum_{ij} C_{ij}(\sigma_i\otimes\sigma_j)\right) \quad (5)$$

and we derive single-qubit maps using Eq. (4). From this, we find the inequality

$$|\sin\theta(B_z\sin\theta + C_{xx}\cos\theta + C_{yy}\cos\theta)| + |\cos^2\theta| \leq 1 \quad (6)$$

determines if a map is CP or not. Using this, we produce the following simulations:

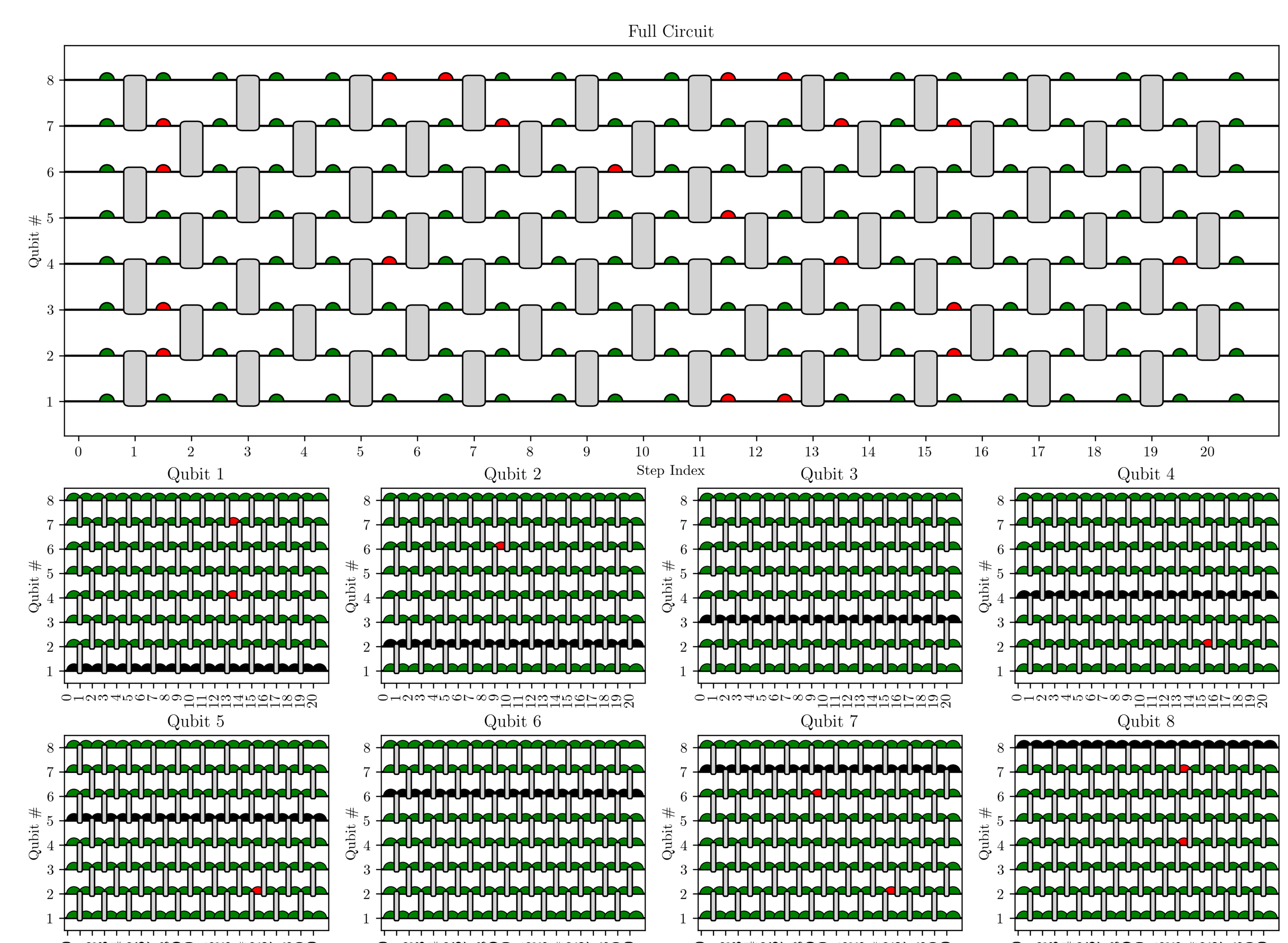


Figure 3. The top figure displays which of the single qubit maps Λ_i are CP after a unitary is applied between pairs. The subplots display whether the map derived for qubit i applied to the state of qubit $j \neq i$, $\Lambda_i\rho_j$, results in a valid state.

Extracting Thermodynamic Properties from the Simulation

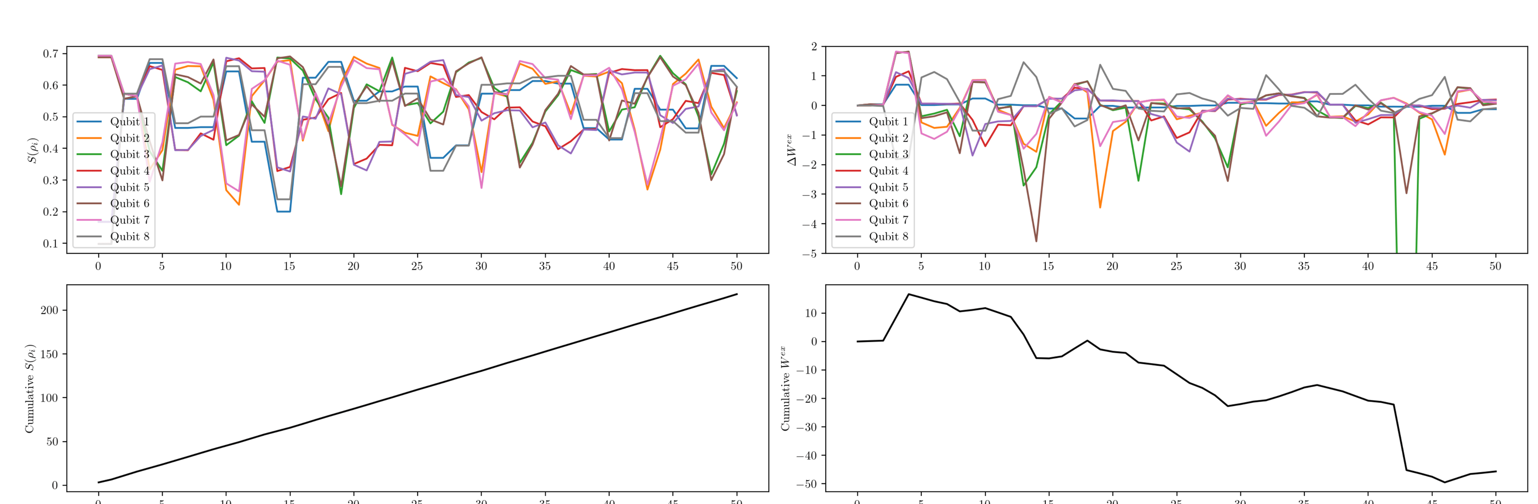


Figure 4. Tracking $S(\rho_i)$ and $\Delta W^{\mathrm{ex}}(\rho_i)$ and their accumulation over the simulation.

From these simulations, we can define thermodynamic properties and track these quantities over time. We first define the Von Neumann entropy:

$$S(\rho_j) = -\sum_i \lambda_i \ln(\lambda_i) \quad (7)$$

where λ_i are the eigenvalues of ρ_j. The free energy is defined as:

$$\mathcal{F}_{\mathrm{sys}} = p_{\mathrm{sys}}^{(i)} - \frac{S(\rho_{\mathrm{sys}})}{k_B \ln\left((1-p_{\mathrm{sys}}^{(i)})/p_{\mathrm{sys}}^{(i)}\right)} \quad (8)$$

and we track the evolution of $\Delta W^{\mathrm{ex}} := \mathcal{F}_{\mathrm{sys}} - \mathcal{F}_{\mathrm{env}}$.

Probing Entanglement

One measure of measuring the correlations between subsystems motivated by classical information theory is mutual information, defined as

$$I(A:B) := S(\rho_A) + S(\rho_B) - S(\rho_{AB}). \quad (9)$$

We define this property for each qubit pair and track its evolution over the simulation. The following is one method of visualizing this quantity:

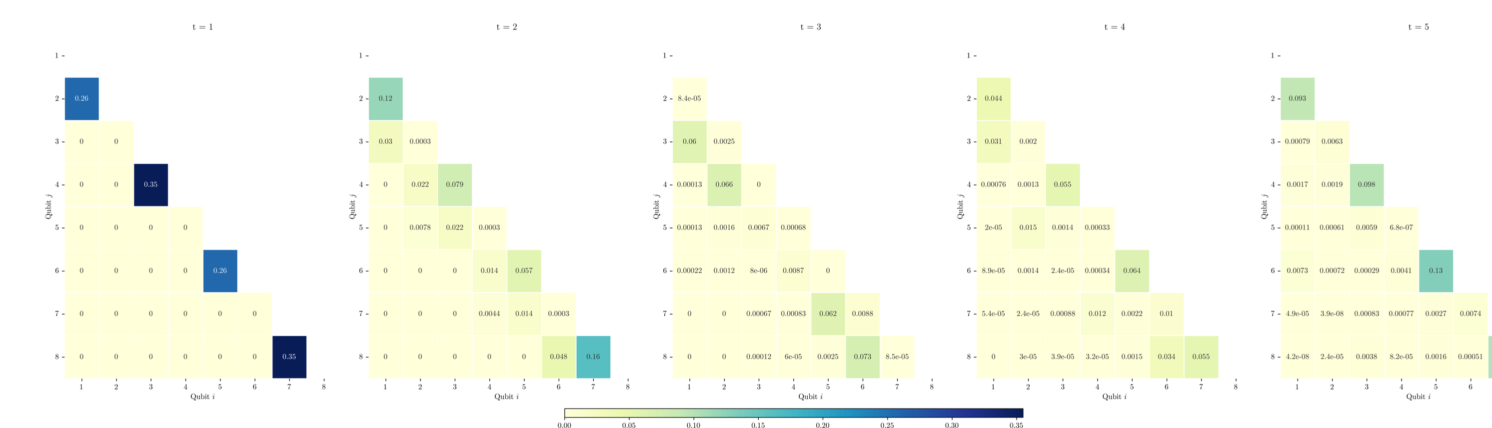


Figure 5. Visualizing the spread of mutual information for the simulation show in Fig. 3.

Mutual information and connectivity are both quantities that are best visualized in the network animations We also study the evolution of concurrence over the circuit and look for its coincidences with the arrival of NCP maps.

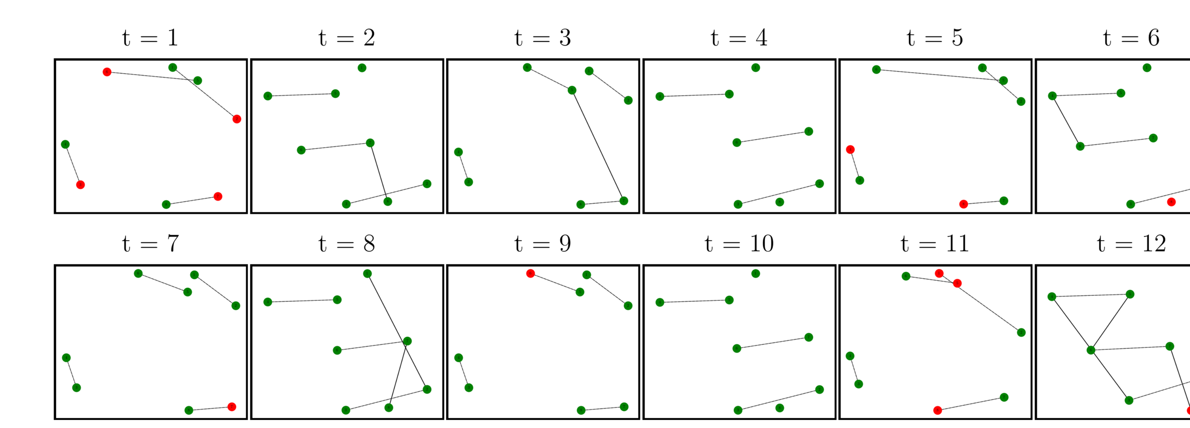


Figure 6. Snapshots from one of the concurrence network animations generated.

Comparing the Evolution Across Varied Circuits

We first compare the evolution for varying deviations in the initial excitation levels:

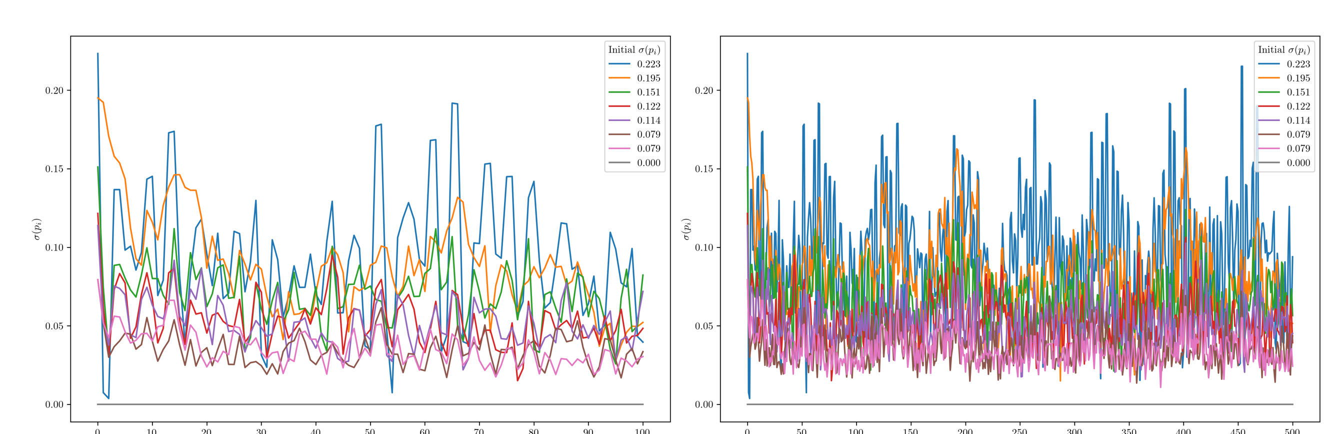


Figure 7. Tracking the deviation in energy levels of individual qubits over the simulation. Notice the grouping present in the first plot and the recurrence in the second. The difference in the $\sigma(p_i)$ repeat is due to the placement of the qubit with unequal excitation within the circuit.

We also compare the evolution under the unitary shown in Eq. (4) and a random Haar unitary:

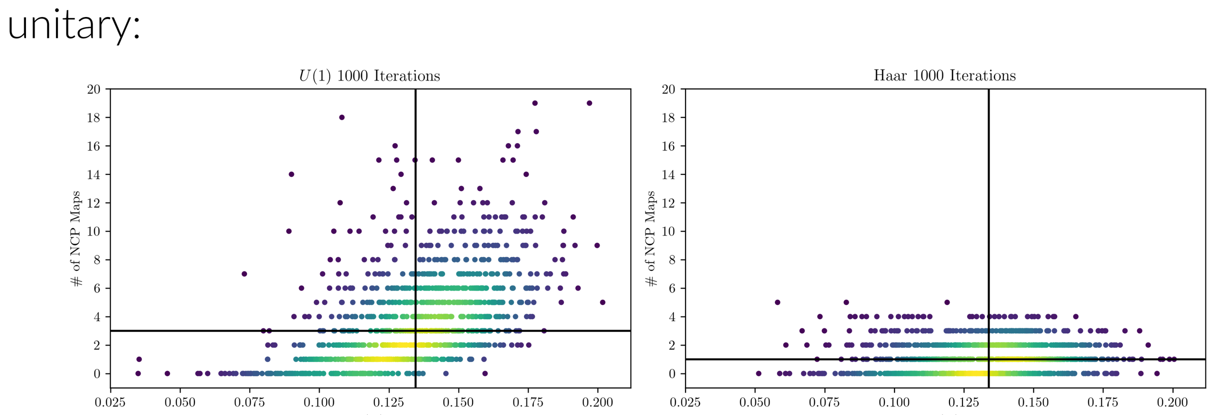


Figure 8. Comparing the number of NCP maps appearing for $U(1)$ and Haar unitaries over 1000 iterations for each. The black lines represent the median of the respective quantity.

Conclusions and Future Work

A correlation between the arrival of NCP maps and the properties we track over the circuit is not immediately apparent with the techniques shown in this poster. We will continue to search for the relationship between NCP maps and signs of higher order entanglement in the future. Machine learning algorithms may also be applied to the data being generated by the simulations.

References & Acknowledgements

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[1] Jagadish, V., & Petruccione, F. (2018). An Invitation to Quantum Channels. Quanta, 7(1), 54-67