Proposing Two New Sets of Decomposable Entanglement Witnesses for Adaptive Measurement Protocol

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Abstract

Quantum entanglement can be utilized for quantum information applications, super dense coding, and secure communications. Understanding whether a state is entangled is imperative for both near and far term quantum cryptography and communication. An entanglement witness is an observable whose expectation value becomes negative only for entangled states. We introduce two new sets of entanglement witnesses, the $\{V\}$ and $\{W''\}$, to an existing adaptive entanglement measurement protocol. We place limits on the existence of decomposable entanglement witnesses. We are interested in maximizing the probability of witnessing entanglement with a limited number of measurements on multiple copies of our entangled pair.

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Chapter 1

Introduction and Background

1.1 Introduction

Understanding how entanglement changes over time and space is essential to many quantum computing and communications applications. Entangled pairs of particles or photons that cannot be measured simultaneously pose a particular challenge. In many quantum communication applications, entangled pairs of photons are separated over long distances. Receivers only have access to one of two in an entangled pair. Different methods to characterize entanglement with access to only one particle in separated entangled pairs (locally correlated entanglement) are necessary to enable quantum communication.

Quantum entanglement witnessing is one method that uses locally correlated measurements to determine two-qubit entanglement. In experiments that use entanglement witnessing, one sender, Alice, forwards pairs of identical entangled photons to two receivers, Bob and Charlie. Bob and Charlie, each receiving only one of the two photons, want to know quickly and accurately whether their photon is *really* entangled with the other photon in the pair. In order to do this, Bob and Charlie must make some set of measurements on their photons alone. Bob and Charlie must continue to measure many photons to keep up with Alice as she continues to send pairs, and communicate with each other classically to put together their information about their entangled pairs. There are myriad problems that may arise for Bob and Charlie: the photons they receive from Alice may have become entangled with the environment along their journeys, or maybe Alice's own transmission apparatus is not as good at producing entangled states as Alice initially suspected. At the end of the day, Bob and Charlie must measure their individual photons to gain any information about entanglement or the issues with transmission.

Entanglement witnesses provide a way to understand the locally correlated measurements made by Bob and Charlie. Without Bob and Charlie taking too many measurements, entanglement witnesses help determine whether the photons sent by Alice are truly entangled. The key question is: how much information about the exchanged photons can Bob and Charlie get with the fewest number of measurements? This thesis addresses this question, and proposes additional entanglement witnesses to probe this balance.

1.2 Background

1.2.1 Measurement, Qubits, and Expectation Values

In the Quantum Optics lab, we make use of photon polarization states for our qubits. We use a horizontally or vertically polarized photon as an excited or ground state qubit. We have the basis states:

$$|H\rangle = |0\rangle \,, |V\rangle = |1\rangle$$

Measurement and expectation values in the physical photon-measuring apparatus are obtained by sending photons into a photodetector. We can do different measurements by changing orientation of half-waveplates, and getting different photon states in two detectors. For more details, see Scholin et al. (2023).

For the purposes of this thesis, we find expectation values of different operators by simulating entangled states in the H, V basis, and measuring them using the density matrix formalism. In the lab, this would require producing many photons and taking measurements with a photodetector.

This thesis also makes ample use of two-qubit pairs without considering how photons are distributed in the lab. However, these states, like in the state $|HH\rangle$, are produced on our apparatus in the lab. In our lab and in the context of locally correlated measurements, we never measure both qubits as one system. Instead, we have physical separation between each qubit in this pair. So, in order to obtain information about entanglement, we must do repeated measurements on one qubit in many identical states produced by our apparatus. In the theoretical calculations, we only need one ket to calculate expectation values. However, in the lab, there are many more complications about which photons we produce. Read more about mixed states below to understand the implications of this.

1.2.2 Pauli Operators

This thesis makes ample use of the Pauli matrix basis. This set of matrices forms a basis for any set of 2×2 operations. We usually write them in the z basis: that is, in the basis of the eigenvectors of the σ_z operator. The z basis in our apparatus is: $|H\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|V\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. The matrices in this basis are given below:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

This basis set is orthogonal, and is useful for single-qubit operations. We can also create 16, 4×4 matrices by considering tensor products of these matrices. These tensor product pairs are useful for two-qubit systems. This set of 4×4 matrices is a basis for all possible 4×4 matrices. An example is the $\sigma_x \otimes \sigma_z$ matrix:

$$\sigma_x \otimes \sigma_z = \begin{pmatrix} 0 \times \sigma_z & 1 \times \sigma_z \\ 1 \times \sigma_z & 0 \times \sigma_z \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

We can find all other combinations of pauli matrix pairs this way (i.e. $\sigma_0 \otimes \sigma_0$, $\sigma_0 \otimes \sigma_x$ ...). This is the basis used for many of the calculations in this thesis. For more detail on these matrices, see section 4.3.

1.2.3 Bell States

Bell states are a specific set of two-qubit entangled states. They are the 'most entangled' that a set of qubits can be. They also can be written in any basis, which can be deduced from the definition of entanglement. These follow the standard conventions:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|HH\rangle + |VV\rangle)$$

$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}(|HH\rangle - |VV\rangle)$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|HV\rangle + |VH\rangle)$$

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|HV\rangle - |VH\rangle)$$

These are useful as a basis for two-qubit states. They are also produced physically by our apparatus.

1.2.4 Density Matrices and Mixed States

Density matrices are an alternate method of describing quantum states to braket notation. These are useful because they allow you to describe mixed states - quantum states that are a mixed ensemble of different pure states. In the lab, mixed states are what is actually produced by our apparatus. If we don't exactly produce the state that we believe we produce 100% of the time, we mathematically describe this with a mixed state. If some of the many photons that we produce have a state that changes in time or get entangled with some other particles, we need a mixed state. Though this thesis makes use of plenty of pure states, the final goal is to detect entanglement in arbitrary mixed states. To do this, we need a density matrices.

Density matrices are exactly the probabilistic mixture we desire. We create them from kets:

$$\rho = \sum_{i=0}^{n} p_i |\psi_i\rangle \langle\psi_i|$$

Where we can sum over all n states in our ensemble and the probabilities of getting them.

We can do everything with density matrices that we could do with braket notation. For this thesis, it is useful to know that we get the expectation value of some operator $\hat{O}$:

$$\langle O\rangle = tr(\rho\hat{O})$$

And that, for all density matrices, $tr(\rho) = 1$. Something similar occurs with $tr(\rho^2)$. But $tr(\rho^2) \leq 1$, where it is only 1 for a pure state.

Much like with pure states, if we know a state's density matrix, we can fully describe the state. As will be discussed in the next chapter, a full state tomography of a two-qubit entangled state amounts to learning the density matrix. If we can find the density matrix, we can determine whether or not our state is entangled. For more in-depth information on density matrices and how to determine entanglement from them, see Lynn (2021).

Chapter 2

Entanglement Witnesses

This chapter details how entanglement witnesses are formulated, and describes two specific sets of entanglement witnesses that the Quantum Optics group uses to witness entanglement.

2.1 State Tomography

There are multiple ways to characterize entanglement with locally correlated measurements, but all rely on classical combinations of individual photon measurements. To verify entanglement with complete certainty, one needs to take a full 'quantum tomography' of the entangled photons. A quantum tomography is a full characterization of the quantum state: a tomography requires taking all the measurements to reconstruct a state in full, using an ensemble of identical states (Purakayastha (2024)). To describe a seperated two-qubit state, we can use the Pauli measurement basis 1.2. In order to take a full quantum tomography, we must measure each photon of a photon pair in all combinations of x, y, and z bases possible. Since we describe each photon in the pair using these bases, the overall tomography takes measurements in 9 bases. In addition, correlations between one photon state and identity (i.e. just measuring the photon on its own) are part of the tomography. The photon correlations with the identity are already covered by our previous measurements since we take individual measurements on each photon and classically combine statistics after measurement. Definitively, if a quantum state is correlated in all bases, it is entangled.

The trick is that a full state tomography can be an arduous process. In one recent experiment, doing the full tomography after transporting entangled photons over long distances takes 160 hours for each measurement Liu et al. (2021). For cryptography or algorithms, this is far too much overhead to complete in future industrial computing applications.

Entanglement witnessing offers an alternative to a full quantum tomography. Rather than complete the 9 measurements required for a full quantum tomography, entanglement witnesses are able to find entanglement with only a subset of the 9 bases measurements required. In this chapter, we explore entanglement witnesses defined by Riccardi et al. (2020), as well as the Quantum Optics group's own set of proposed witnesses Yang et al. (2022).

2.2 Entanglment Witnesses

2.2.1 Entanglement Witnessing

An entanglement witness is an operator such that a negative expectation value implies the presence of entanglement in a quantum state. More mathematically, for an entanglement witness W, if $Tr[\rho W] < 0$, ρ has at least one entangled state Riccardi et al. (2020). In other words, if the state is not entangled, the expectation value of the entanglement witness operator for that state is positive.

To explain how entanglement witnesses work, let's quickly create our own to find entanglement in these states: we have a laser that produces pairs of photons with state $|HH\rangle$ half the time, or $|VV\rangle$ half the time. This looks like a density matrix

$$\rho_{sep} = \begin{pmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.5 \end{pmatrix}$$

We have a second laser that produces only $|\Phi^+\rangle$ states. These states have a density matrix that look like

$$\rho_{ent} = \begin{pmatrix} 0.5 & 0 & 0 & 0.5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0.5 \end{pmatrix}$$

An entanglement witness operator, W_{ex}, will tell us that laser one is only producing pairs of correlated photons, while laser 2 is producing pairs of entangled photons. Let's define a witness:

$$W_{ex} = \begin{pmatrix} 0 & 0 & 0 & -0.5 \\ 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & 0 \\ -0.5 & 0 & 0 & 0 \end{pmatrix}$$

Sure enough, this operator acts as we wish. $tr(\rho_{sep} W_{ex}) = 0$, while $tr(\rho_{ent} W_{ex}) = -1$. Notice even $tr(\frac{1}{2}(\rho_{sep} + \rho_{ent}) W_{ex}) = -1$, because if a density matrix has just one entangled pure state, an entanglement witness can witness it. It would be lovely if we could engineer an entanglement witness like this every time we needed to, for every individual set of states. However, for an arbitrary state in the lab, we don't know what our state density matrix looks like. In the lab, we have some mixed state density matrix, $\rho_{mystery}$. $\rho_{mystery}$ can consist of an ensemble of states, some entangled and others not. We would like to know, for one of those arbitrary mixed states, whether there is any entanglement. This means doing some process like $tr(\rho_{mystery} W_{ex}) =?$ for different states, with different entanglement witnesses.

An entangled state may have an expectation value from a witness that is greater than 0. This does not rule out the presence of entanglement. Our definition of an entanglement witness only states a negative expectation value promises entanglement, but a positive one does not rule out entanglement. In the case we do have a positive expectation value on an entangled state, the witness 'missed' that state. For an entangled state, we hope this doesn't happen often. Missed states are the drawback of entanglement witnessing. In a full quantum tomography, we know for certain whether entanglement is present after finishing all our measurements. Entanglement witnessing constructs an operator of a subset of the measurements required for a full tomography, and gets a fairly accurate idea of entanglement in the state.

An effective set of witnesses will take a smaller fraction of measurements than the information payoff about entanglement from those measurements. For example, imagine an entanglement witness that could take 3/9 of measurements required for a full quantum tomography, and result in witnessing 45% of entangled states. Of course, even in this example, 55% of entangled states will be 'missed'. Entanglement witnesses trade a lower number of measurements for possible inaccuracy in characterizing entanglement.

2.2.2 The W Witnesses

The Quantum Optics group began the investigation of entanglement witnessing by taking inspiration from a paper published by Riccardi et al. (2020). This paper introduced a set of entanglement witnesses that could be created by taking the partial transpose of a density matrix of just one entangled pure state. As introduced by Riccardi et al. (2020), these decomposable, extremal witnesses are what we call the Ws. We call a witness *decomposable* if we can write $W = |\psi\rangle\langle\psi|^{\Gamma}$, where $|\psi\rangle$ is some entangled state. The Γ operator is the partial transpose over the matrix produced by the outer product, with respect to the second qubit. See Lynn (2021) for further mathematical detail.

Considering only measurements between the same pairs of pauli matrices (i.e. $\sigma_k \otimes \sigma_k$ where $k = x, y, z$) Riccardi et al. (2020) finds a set of decomposable entanglement witnesses of this form. The W set is defined by the original 6 separable states such that $W_k = |\varphi_k\rangle\langle\varphi_k|^{\Gamma}$. These states are given by equation 2.1.

$$\begin{aligned} |\varphi_1\rangle &= \cos\theta\,|\Phi^+\rangle + \sin\theta\,|\Phi^-\rangle & |\varphi_2\rangle &= \cos\theta\,|\Psi^+\rangle + \sin\theta\,|\Psi^-\rangle \\ |\varphi_3\rangle &= \cos\theta\,|\Phi^+\rangle + \sin\theta\,|\Psi^+\rangle & |\varphi_4\rangle &= \cos\theta\,|\Phi^-\rangle + \sin\theta\,|\Psi^-\rangle \\ |\varphi_5\rangle &= \cos\theta\,|\Phi^+\rangle + i\sin\theta\,|\Psi^-\rangle & |\varphi_6\rangle &= \cos\theta\,|\Phi^-\rangle + i\sin\theta\,|\Psi^+\rangle \end{aligned} \tag{2.1}$$

θ can be varied for each of these 6 states to produce a full family of witnesses. Of the measurement bases required for a full quantum tomography, these witnesses take 3/9: $\sigma_x \otimes \sigma_x, \sigma_y \otimes \sigma_y, \sigma_z \otimes \sigma_z$. The pauli matrix formulation of these witnesses is given below:

$$
\begin{aligned}
W_1 = &\frac{1}{4}[\mathbb{I} \otimes \mathbb{I} + \sigma_z \otimes \sigma_z + (\cos\theta^2 - \sin\theta^2)\sigma_x \otimes \sigma_x + (\cos\theta^2 - \sin\theta^2)\sigma_y \otimes \sigma_y \\
&+ 2\cos\theta\sin\theta(\sigma_z \otimes \mathbb{I} + \mathbb{I} \otimes \sigma_z)] \\
W_2 = &\frac{1}{4}[\mathbb{I} \otimes \mathbb{I} - \sigma_z \otimes \sigma_z + (\cos\theta^2 - \sin\theta^2)\sigma_x \otimes \sigma_x + (\cos\theta^2 - \sin\theta^2)\sigma_y \otimes \sigma_y \\
&+ 2\cos\theta\sin\theta(\sigma_z \otimes \mathbb{I} + \mathbb{I} \otimes \sigma_z)] \\
W_3 = &\frac{1}{4}[\mathbb{I} \otimes \mathbb{I} + \sigma_x \otimes \sigma_x + (\cos\theta^2 - \sin\theta^2)\sigma_z \otimes \sigma_z + (\cos\theta^2 - \sin\theta^2)\sigma_y \otimes \sigma_y \\
&+ 2\cos\theta\sin\theta(\sigma_x \otimes \mathbb{I} + \mathbb{I} \otimes \sigma_x)] \\
W_4 = &\frac{1}{4}[\mathbb{I} \otimes \mathbb{I} - \sigma_x \otimes \sigma_x + (\cos\theta^2 - \sin\theta^2)\sigma_z \otimes \sigma_z - (\cos\theta^2 - \sin\theta^2)\sigma_y \otimes \sigma_y \\
&- 2\cos\theta\sin\theta(\sigma_x \otimes \mathbb{I} + \mathbb{I} \otimes \sigma_x)] \\
W_5 = &\frac{1}{4}[\mathbb{I} \otimes \mathbb{I} + \sigma_y \otimes \sigma_y + (\cos\theta^2 - \sin\theta^2)\sigma_z \otimes \sigma_z + (\cos\theta^2 - \sin\theta^2)\sigma_x \otimes \sigma_x \\
&+ 2\cos\theta\sin\theta(\sigma_y \otimes \mathbb{I} + \mathbb{I} \otimes \sigma_y)] \\
W_6 = &\frac{1}{4}[\mathbb{I} \otimes \mathbb{I} - \sigma_y \otimes \sigma_y + (\cos\theta^2 - \sin\theta^2)\sigma_z \otimes \sigma_z - (\cos\theta^2 - \sin\theta^2)\sigma_x \otimes \sigma_x \\
&- 2\cos\theta\sin\theta(\sigma_y \otimes \mathbb{I} + \mathbb{I} \otimes \sigma_y)]
\end{aligned}
$$

An arbitrarily entangled state can be correlated in other bases besides $\sigma_x \otimes \sigma_x, \sigma_y \otimes \sigma_y, \sigma_z \otimes \sigma_z$. The set of W witnesses misses a significant number of entangled states that are correlated in other bases. The Quantum Optics group found in 2022 that the W miss 66% of all entangled states that were generated randomly via a method laid out in Roik et al. (2021).

Taking one or two more sets of measurements can help determine whether a state is entangled, beyond the 3 that are taken by the $\{W\}$. We notice that the Ws witness random entangled states in a 1:1 ratio with the proportion of measurements they require: $3/9$ measurements for a full quantum tomography corresponds to witnessing 33% of the mixed states. The Quantum Optics group decided that taking more measurements like the W could extend the 1:1 ratio, or improve upon it. To add more measurements, the Quantum Optics lab chose to define more witnesses that come closer to achieving the amount of information gained by a full quantum tomography. These witnesses require more combinations of bases measurements: they are not be confined to measuring correlation in the same bases for both photons. This new set of witnesses is described in the following section.

2.3 The W′ Witnesses

To consider correlations in different combinations of photon basis, we must introduce new witnesses. The set of separable witnesses the Quantum Optics group introduced to extend the W are called the W' set in Yang et al. (2022). They take the same form as the W, so that an entangled state φ'_k makes the kth W': $W'_k = \left|\varphi'_k\right\rangle \left\langle\varphi'_k\right|^{\Gamma}$. The full set of W' states is given in Yang et al. (2022), but the ket formulation of the witnesses is displayed here below.

$$
\begin{aligned}
&\left|\varphi'_1\right\rangle = \cos\theta \left|\Phi^+\right\rangle + e^{i\alpha}\sin\theta \left|\Phi^-\right\rangle \\
&\left|\varphi'_2\right\rangle = \cos\theta \left|\Psi^+\right\rangle + e^{i\alpha}\sin\theta \left|\Psi^-\right\rangle \\
&\left|\varphi'_3\right\rangle = \frac{1}{\sqrt{2}}(\cos\theta \left|HH\right\rangle + e^{i(\beta-\alpha)}\sin\theta \left|HV\right\rangle + e^{i\alpha}\sin\theta \left|VH\right\rangle + e^{i\beta}\cos\theta \left|VV\right\rangle) \\
&\left|\varphi'_4\right\rangle = \cos\theta \left|\Phi^+\right\rangle + e^{i\alpha}\sin\theta \left|\Psi^+\right\rangle \\
&\left|\varphi'_5\right\rangle = \cos\theta \left|\Phi^-\right\rangle + e^{i\alpha}\sin\theta \left|\Psi^-\right\rangle \\
&\left|\varphi'_6\right\rangle = \cos\theta\cos\alpha \left|HH\right\rangle + i\cos\theta\sin\alpha \left|HV\right\rangle + i\sin\theta\sin\beta \left|VH\right\rangle + \sin\theta\cos\beta \left|VV\right\rangle \\
&\left|\varphi'_7\right\rangle = \cos\theta \left|\Phi^+\right\rangle + e^{i\alpha}\sin\theta \left|\Psi^-\right\rangle \\
&\left|\varphi'_8\right\rangle = \cos\theta \left|\Phi^-\right\rangle + e^{i\alpha}\sin\theta \left|\Phi^+\right\rangle \\
&\left|\varphi'_9\right\rangle = \cos\theta\cos\alpha \left|HH\right\rangle + \cos\theta\sin\alpha \left|HV\right\rangle + \sin\theta\sin\beta \left|VH\right\rangle + \sin\theta\cos\beta \left|VV\right\rangle
\end{aligned}
$$

The states that produce the W' allow measurement of correlations across new combinations of pauli matrix bases: the $\sigma_x \otimes \sigma_y, \sigma_x \otimes \sigma_z, \sigma_y \otimes \sigma_x, \sigma_y \otimes \sigma_z, \sigma_z \otimes \sigma_y, \sigma_z \otimes \sigma_x$. Adding these to the set of measurements required for the W set, the W' set considerably widens the range of possible entangled states that can be detected by the combination of measurements. In fact, the Summer 2023 Quantum Optics team found that an ideal picking of a subset of W', in addition to the measurements done by W, results in missing only 22% of entangled states in Scholin et al. (2023). The process of picking and the witness subgroups are detailed in the next chapter.

Performing all the W and W' measurements would amount to a full quantum tomography. As we have seen, this is the very process that entanglement witnessing seeks to avoid. Rather than complete a full quantum tomography, our lab makes use of a two-step process, described in the next chapter.

Chapter 3

Picking Witnesses

The process of picking witnesses is key to capitalize on the power of entanglement witnessing. We could just randomly sample measurements from our set of 9, and hope that a combination of measurements witnesses entanglement before we complete a full quantum tomography. This could work sometimes. However, picking our measurements strategically to cover the most optimal basis combinations given our random state will raise our chances of witnessing entanglement, with fewer measurements.

We would like to witness entanglement with as few measurements as possible. In order to do this, we must come up with some method to strategically pick our measurements based on our state. To make an informed decision about the measurements to pick, we must have an idea about the entanglement of a state, or else we would simply hope to get lucky. This framing of our problem seems circular: to get information about a state, we must know information about it? The Quantum Optics group has provided a way around this problem. We call our witness picking protocol the ’two step process’, and it endeavors to use information about entanglement from one set of witnesses to pick another set of witnesses.

This chapter details the two-step process, and explains how witnesses are subdivided for easy picking. The efficacy of current witness groups is also discussed and displayed. The states that are missed by the current two step process (the ’unwitnessed states’) are described.

3.1 The Two-Step Process

The two-step process uses measurements that find W expectation values to pick which measurements to perform that find W' expectation values. There are also two parts to the two-step process protocol: a before lab component, and an in-lab component.

3.1.1 Pre-Lab Component

The general idea of the two-step process works like this. Rather than complete all measurements for all W and W' witnesses at once, we first find the expectation values of all the W witnesses for a random mixed state. If any of these expectation values is negative, the whole two step process terminates, and returns that the state we are characterizing is entangled. If none of the $\{W\}$ set find that the state is entangled, the process moves to the second stage. Using the information from the W expectation values, we pick a subset of 3 W' witnesses that are most conducive to fully characterizing system entanglement. Based on this choice of 3 of the 9 $\{W'\}$, we get the expectation values of each of these W'. From these 3 witnesses, if any of the W' subset find entanglement, the two step process returns that the state is entangled. Otherwise, it does not find entanglement.

The pre-lab component of this process enables us to pick a subset of W' quickly in the lab. Before any experiment is done, we train a neural network, as crafted in Scholin et al. (2023). To train the neural network, we generate a set of random entangled states by the method laid out in Roik et al. (2021). For each of these entangled states, we find the W expectation values. We use the output of the neural network to pick the W' subset to try on our randomly generated state. Since the random states are computationally generated, we have access to their full density matrix. Therefore, we can determine whether a randomly generated state is entangled or not, and check it against the witness expectation values of the W' subgroup from the neural network. We train the neural network by iterating through these random states.

3.1.2 In-Lab Component

The in-lab component of the two-step process uses the trained neural network. After finding real expectation values from the W pauli matrix component measurements, we feed our measurement results into the trained neural

$\sigma_x \otimes \sigma_x$	$\sigma_x \otimes \sigma_y$	$\sigma_x \otimes \sigma_z$
$\sigma_y \otimes \sigma_x$	$\sigma_y \otimes \sigma_y$	$\sigma_y \otimes \sigma_z$
$\sigma_z \otimes \sigma_x$	$\sigma_z \otimes \sigma_y$	$\sigma_z \otimes \sigma_z$

Table 3.1 W' subgroup categories from full quantum tomography. The light blue colored entries indicate that those measurements are required for the original W subgroup, proposed by Riccardi et al. (2020). The purple cells are measurements that go into the W'_{1-3} subgroup, the pink are measurements that are required for W'_{4-6}, and the green are measurements required for W'_{7-9}. The W' subgroups do not mix: including a measurement from another color of subgroup would amount to proposing a new witness set.

network. The neural network's output determines which subgroup of W' we pick to try and witness our state in real time. The measurements that we complete in addition to the W measurements are picked by the neural network.

Yet again, it is possible that entanglement is still not detected. Detecting entanglement with certainty requires a full quantum tomography. Since a full quantum tomography would require all the subgroups of W's, the neural network cannot always pick the correct subset that will characterize entanglement. Though the two-step process works most of the time, there are still states that are not picked up by both the $\{W\}$ measurements and a subset of the $\{W'\}$ measurements. More detail into these states, as well as the strategy for implementing new measurements to catch these states, is described in section 3.3.

3.2 Efficacy of Witness Groups

The efficacy of each of the witness groups, $\{W\}$ and $\{W'\}$, is displayed in figure 3.1. The addition of 2 carefully selected measurements improves the accuracy of the the W entanglement witnessing immensely. The $5/9$ measurements required for a full quantum tomography witness more than $2/3$ of the randomly generated states.

3.2.1 Flaws in the Two-Step Process

Noticeably, the different methods for picking W' subgroups converge at a similar detection success in the left plot of 3.1. This suggests that changing the model we use to pick which W' subgroup is best will not dramatically

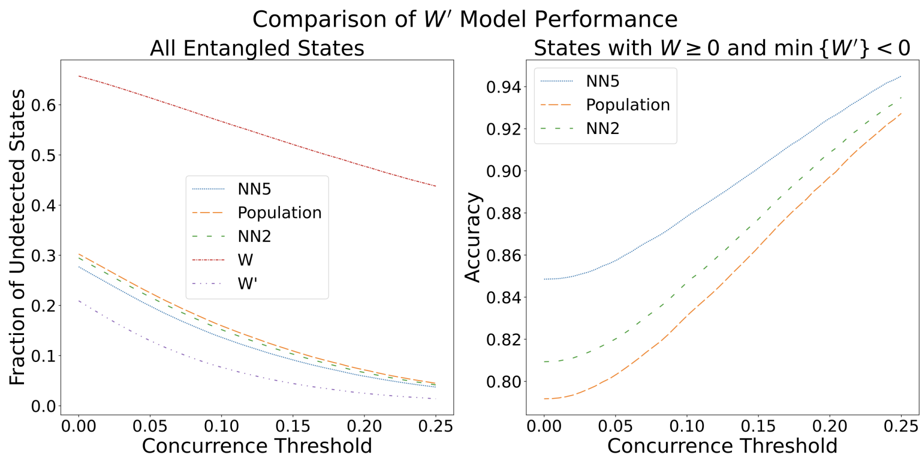

Figure 3.1 The performance of different W' picking models compared. For a randomly generated state, concurrence threshold is the minimum degree of entanglement we want to be able to reliably witness. See original figure and caption in Scholin, Zheng, Roberson, and Lynn (Left) The fraction of states not detected by W' and W with various selection methods. 'NN5' is a 5-layer neural network, 'NN2' is a 2-layer neural network, and 'Population' is an analytical picking method developed in Yang et al. (2022). The W line is the proportion of states that remain undetected by the W at various degrees of entanglement. The W' method represents an ideal scenario where the W' subgroup selector always picks the correct W' subgroup to witness a random state. With concurrence threshold 0, the W witnesses do not detect $\frac{2}{3}$ of randomly generated states. The W', with a subgroup picked via the methods labelled, do not witness 28% of states. However, via the method labelled W', only 21% of states are not witnessed. (Right) The accuracy of the W' in detecting a state missed by W for various W' picking methods. Each label refers to the method used to pick the W' subgroup to witness the state. The selection methods are the same as on the left panel, excluding the ideal W' picking method. A W' subgroup witnesses 85% of entangled states that were missed by W, but could be witnessed by at least one W'.

change the detection success. We may require more information to improve our W' picking technique. All these different methods are about 10% success detection away from convergence with the maximum possible, the ideal W' picker. These methods may need to be improved in the future, but improving their accuracy will likely not result in the highest possible information return.

Instead, consider the ideal possible W' subgroup picker in figure 3.1. This W' picker indicates that, no matter the method, $1/5$ of randomly generated entangled states will go unwitnessed by W' witnesses. The goal of the remainder of this thesis is to then lower the percentage of W' that go unwitnessed in this ideal scenario. We seek to first re-allocate the W' groups that we pick from. The W' picker line could be lowered by changing the possible picking options in step two of the two step process. We hope to allow our two-step process to pick two pauli matrix measurement combinations, independent of their W' subgroup. We try to find combinations of two pauli matrix measurements that can act as alternatives to the W' in the second stage of the two-step process. It turns out to be impossible to create more witnesses with just two pauli basis measurements. Instead, we advise adding additional witness subgroups to collect more information. First, as is detailed in section 3.3, we explore the witness states that are missed by W' to gain insight for new possible measurement allocation groups.

3.3 Unwitnessed States and Ways to Witness Them

3.3.1 Unwitnessed States

Despite the new expanded set of pauli basis measurements necessary for the two-step process, there are still many unwitnessed entangled states. Since the full set of $\{W\}$ and $\{W'\}$ would amount to a full quantum tomography, there would not be any missed states by running all possible measurements. However, there are some consistently missed states in the two-step process. Among these are states that are entangled *between* bases that make up the measurements for different W' subsets. For example, as shown in table 3.2, the $\{W\}$ set handles correlations between $|H\rangle$ and itself, and the group of W'_{4-6} handles correlations between $|H\rangle$ and $|R\rangle$ bases. However, there are some sets of states that are most correlated between these two bases. The set of states with the form $|\psi\rangle = \frac{1}{\sqrt{N}}(|HR\rangle + e^{i\theta}|RH\rangle)$ (where N is some normalization factor and θ is some phase) are consistently missed in the two-step process.

HH, HV, VH, VV	RD, RA, LD, LA	HD, HA, VD, VA
DR, DL, AR, AL	DD, DA, AD, AA	RH, RV, LH, LV
HD, HA, VD, VA	HR, HL, VR, VL	RR, RL, LR, LL

Table 3.2 The light blue color indicates physical basis combination measurements needed by the W on each photon in the experiment. The purple is the measurements for W'_{7-9}, the green is for W'_{4-6}, and the red for W'_{1-3}. This table 'matches' table 3.1, but shows the in-lab measurements required to perform analysis.

3.3.2 States and Corresponding Witnesses

These missed states beg the question: which witnesses catch which states? It turns out that in the set of Ws, we find that the most *opposite* witnesses to an entangled state have a negative expectation value. To see why, we can investigate the partial transpose. Suppose we are given an entangled state:

$$\left|\Psi^+\right\rangle = \frac{1}{\sqrt{2}}(|HV\rangle + |VH\rangle)$$

This state will be witnessed by the Ws. All the witnesses in W that have a most opposite bell state - i.e. $|\Phi^-\rangle$ - most effectively witness this state. In fact, this was the first example of entanglement witnessing presented in this thesis, in section1.2. In this example, without knowing it, we found that because the partial transpose sent $|HV\rangle\langle HV| \rightarrow |HH\rangle\langle VV|$, our entangled state was witnessed. In the W, this rule generally holds - the partial transpose allows the opposite sign, opposite bell state type (symmetric or anti-symmetric) to witness each other. The sign must be opposite because overall we want a negative expectation value. The symmetry must be opposite so that there is a non-zero product between a witness matrix and density matrix. We denote this pattern of witnessing states the 'most opposite' or the most 'opposite Bell state' to witness some state.

So our example bell state ($|\Psi^+\rangle$) should be witnessed by W_1, W_4 and W_6 since those contain $|\Phi^-\rangle$. The distribution of the witnesses (the optimization) also puts more weight on the component of the witnesses containing the opposite bell state. For an example witness state like $\left|\phi_k\right\rangle = a\,|\Phi^+\rangle + b\,|\Phi^-\rangle$, the b value for all the witnesses should be maximized and the a value should be minimized. We can compute the expectation value using density operator formalism for the example with $\rho = |\Psi^+\rangle\langle\Psi^+|$ and W_1. The density operator

ρ is then:

$$\rho = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{3.1}$$

And W_2, with arbitrary a and b yet to be optimized, is given by:

$$W_1 = ((a\left|\Phi^+\right\rangle + b\left|\Phi^-\right\rangle)(a\left\langle\Phi^+\right| + b\left\langle\Phi^-\right|))^\Gamma \tag{3.2}$$

Which gives us the matrices:

$$\frac{1}{2}\begin{pmatrix} (a+b)^2 & 0 & 0 & a^2-b^2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ a^2-b^2 & 0 & 0 & (a-b)^2 \end{pmatrix}^\Gamma = \frac{1}{2}\begin{pmatrix} (a+b)^2 & 0 & 0 & 0 \\ 0 & 0 & a^2-b^2 & 0 \\ 0 & a^2-b^2 & 0 & 0 \\ 0 & 0 & 0 & (a-b)^2 \end{pmatrix} \tag{3.3}$$

So finally, we are concerned with $tr(\rho W_1)$. This gives us the matrix product:

$$\frac{1}{4}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} (a+b)^2 & 0 & 0 & 0 \\ 0 & 0 & a^2-b^2 & 0 \\ 0 & a^2-b^2 & 0 & 0 \\ 0 & 0 & 0 & (a-b)^2 \end{pmatrix} \tag{3.4}$$

Which we can see will only consider the $a^2 - b^2$ terms from the partial transpose. What's more, we take the trace of this product. This eventually gives us:

$$\langle W_1 \rangle = \frac{1}{2}(a^2 - b^2) \tag{3.5}$$

Upon optimization, we find that our b must be larger than our a to witness our state of interest. This exactly matches our prediction: the most 'opposite' component of our $|\varphi_1\rangle$ ($|\Phi^-\rangle$)to our state $|\Psi^+\rangle$ receives the most weight, and actually does the witnessing.

Generally, the witness that is the 'most opposite' to our state should witness it. This intuition relies on the partial transpose, and will be useful for determining witness subgroups. The full explanation for which witness subgroups exist is detailed in the next chapter.

Chapter 4

Witness Subgroups

As alluded to in prior chapters, in this chapter we will show it is impossible to create witnesses from sets of two pauli basis measurements across the W' subgroups. Based on the intuition built from chapter 3, we might expect that a state that is missed by our two step process would be witnessed by two measurements from two different W' subgroups. Those two measurements would make up a 'most opposite' state. This is not the case. The state is missed because we can't sample only two pauli basis measurements across W' subgroups to make a decomposable witness. The 'most opposite' intuition still holds.

The details for which witness groups *are* allowed are described in this chapter. We describe the limitations on witness groups, and what witness groups are necessary to witness new states. From these investigations, we begin to dive into the emerging structure of a general entanglement witness. Why are some witnesses allowed, and others are not? We begin this discussion, and we present our current understanding of possible witness subgroups.

We also find that constraints on the possible witnesses produce new pauli basis measurement combinations. These new combinations contain three pauli basis measurements instead of two, but witness entangled states that are missed by the existing two-step process.

4.1 The W' Subgroups and Limitations

In the original proposition of the W', the W' naturally fell into three groups. These groups allowed us to witness some state: the state 'most opposite' to that class of witnesses within each subset of measurements. The measurement subsets are shown in photon measurement form in table 3.2, and pauli basis measurement form in 3.1.

4.1.1 States Witnessed by W' Subgroups

Since the W' fall into distinct subgroups, we can directly find what states they should witness. We find that W'_{1-3} use measurements between the diagonal, anti-diagonal and right, left polarized states ($\sigma_x \otimes \sigma_y, \sigma_y \otimes \sigma_x$), the W'_{4-6} use measurements between the horizontal, vertical and right, left polarized states ($\sigma_z \otimes \sigma_y, \sigma_y \otimes \sigma_z$), and W'_{7-9} use measurements between the diagonal, anti-diagonal and horizontal, vertical polarized states ($\sigma_x \otimes \sigma_z, \sigma_z \otimes \sigma_x$), see table 3.2. Using the 'most-opposite' intuition from chapter 3, we would then expect the W'_{1-3} witnesses to also witness states that look like the measurements included in the W'_{1-3}. To see why this is the case, again consider our example entangled state $|\Phi\rangle = \frac{1}{\sqrt{N}}(|HR\rangle + |RH\rangle)$. We can describe this state with the measurements in the W'_{4-6} and W witnesses. The 'most opposite' state would be a negative, partial-transpose version of this state; that is $|\Psi\rangle = \frac{1}{\sqrt{N}}(|HH\rangle - |RR\rangle)$. Since all the measurements for this 'most opposite' state are still in the W'_{4-6} subset, the W and the W'_{4-6} should also witness the most opposite partner state. More generally, we should then expect the W' subgroup that best describes a state to also witness it.

4.1.2 Constructing New Possible Witnesses

As we discovered, each state should be witnessed by the measurements already included in the state. We hope to mix and match the measurements that go into each W' subgroup to create new witnesses. If we would like to witness a state that is not currently witnessed by our various subgroups, we might combine the measurements in the W' subgroups to cover a wider range of state types. We can consider one example that is not witnessed by our current two-step process: our favorite example state, $|\psi\rangle = \frac{1}{\sqrt{N}}(|HR\rangle + i\,|RH\rangle)$, setting our phase factor to $\pi/2$. Our example state combines $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_z$. Not all of the states of this type are missed, but some (like the example $|\psi\rangle$ above) are. If we adhere to our hypothesis that the witness must look like the state it witnesses, a witness candidate must contain *both* $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_z$ to witness states of this type. It is possible to create a witness with $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_z$ using some outer product of a state $|\Psi\rangle = a\,|HH\rangle + be^{i\alpha}\,|HV\rangle + ce^{i\beta}\,|VH\rangle + de^{i\gamma}\,|VV\rangle$. However, we must ask:

along the way, which other pauli measurements did we include? Taking the outer product with such a generic state as $|\Psi\rangle$ will certainly include other pauli measurements besides $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_z$. We need consider what happens to our general state $|\Psi\rangle$ when we wish to include one pauli matrix pair, but not another. Notably, this will allow us to consider groups that have some set of measurements from one W' subgroup, but not another, and possibly even exclude the other measurements in that W' subgroup.

4.2 General Witness Parameterization

We can find the necessary constraints on our pauli measurement combinations by first considering the most generic pure state that can produce any possible witness. Next, we will consider which subsets of possible entangled pure states produce the listed $\sigma_i \otimes \sigma_j$ pairs. This technique will allow us to determine which pauli matrix pairings are allowed to form a witness together.

First, we must note that we are limited to the set of decomposable entanglement witnesses. Any witness containing a pauli matrix pair must be of the form $W = |\psi\rangle \langle\psi|^{\Gamma}$. The most generic pure state that can be turned into a witness is:

$$|\psi\rangle = a\,|HH\rangle + be^{i\beta}\,|HV\rangle + ce^{i\gamma}\,|VH\rangle + de^{i\delta}\,|VV\rangle$$

Where $a^2 + b^2 + c^2 + d^2 = 1$ and all a, b, c and d are real. Then a generic entanglement witness can be expressed by taking an outer product and partial transpose of $|\psi\rangle$.

$$W_{gen} \rightarrow \begin{bmatrix} a^2 & abe^{i\beta} & ace^{-i\gamma} & bce^{i(\beta-\gamma)} \\ abe^{-i\beta} & b^2 & ade^{-i\delta} & bde^{i(\beta-\delta)} \\ ace^{i\gamma} & ade^{i\delta} & c^2 & cde^{i(\delta-\gamma)} \\ bce^{i(\gamma-\beta)} & bde^{i(\delta-\beta)} & cde^{-i(\delta-\gamma)} & d^2 \end{bmatrix} \tag{4.1}$$

From this generic form, we want to know what restrictions lead to witness subgroup pairings; we can explain the W, W', and hopefully create new witnesses along the way. Each combination of pauli measurement pairs has related elements. By including some pauli measurements and excluding others, we can determine what possible witness subsets exist. We can then determine if there are any additional witnesses possible with two, three, or even four measurements drawn from table 3.1.

4.3 Pauli Basis Measurement Pair Subsets

4.3.1 The Partial Transpose and Outer Product

One degree of flexibility we must consider when crafting new witnesses is the partial transpose. The partial transpose is what allowed us to witness an entangled state in section 1.2. It may also place possible limitations on which witness groupings are allowed. After some investigation, we will find that it does neither of these things.

We can consider what happens when we take the partial transpose of our generic entangled state outer product:

$$\begin{bmatrix} a^2 & abe^{-i\beta} & ace^{-i\gamma} & ade^{-i\delta} \\ abe^{i\beta} & b^2 & bce^{i(\beta-\gamma)} & bde^{i(\beta-\delta)} \\ ace^{i\gamma} & bce^{i(\gamma-\beta)} & c^2 & cde^{i(\gamma-\delta)} \\ ade^{i\delta} & bde^{i(\delta-\beta)} & cde^{i(\delta-\gamma)} & d^2 \end{bmatrix}^{\Gamma} \rightarrow \begin{bmatrix} a^2 & abe^{i\beta} & ace^{-i\gamma} & bce^{i(\beta-\gamma)} \\ abe^{-i\beta} & b^2 & ade^{-i\delta} & bde^{i(\beta-\delta)} \\ ace^{i\gamma} & ade^{i\delta} & c^2 & cde^{i(\delta-\gamma)} \\ bce^{i(\gamma-\beta)} & bde^{i(\delta-\beta)} & cde^{-i(\delta-\gamma)} & d^2 \end{bmatrix} \tag{4.2}$$

In this example, the partial transpose exchanges parts of the witness that are covered by the same pauli measurement pairs. That is, were we to model a witness from this state, the partial transpose *would not change any measurements* we need. If we want to witness a state with such a witness, we require entries in our state density matrix to be included in some expectation value. To be included in a trace, these entries need to also be included in the witness.

We must also consider another restriction of our witness type: all decomposable entanglement witnesses can be written in the form $(|\psi\rangle\langle\psi|)^{\Gamma}$. This means that to include some entries in our witness, we may accrue unwanted cross-terms from the outer product when trying to create witness subgroups. In order to witness a state that has pauli matrix components from multiple W' subgroups, we need to include pauli matrix combinations in our witness from multiple different W' subgroups. Since the partial transpose will not introduce any new measurements, the measurements we need to form our density matrix are the same as those to form our witness. In an outer product to create just one pauli matrix pair, we also include the *other* measurements in that outer product. The outer product may force additional cross-terms in our witness that include more measurements than we initially wanted.

We must then ask: what are the limits on the subsets of pauli matrix measurements we can create? If we must sample from multiple subgroups to witness a state composed of measurements from multiple subgroups, we need to limit which subgroups make a witness.

4.3.2 New Pauli Matrix Combinations

Considering which pauli matrix measurement combinations contribute to each entry in our generic entanglement witness is then very useful. Including a pauli matrix in a witness changes the witness entries. We have been categorizing our pauli matrix measurement basis in terms of W' subgroups, but we can now transition to categorizing based on the entries each pauli matrix pair controls in each witness.

We can divide this pauli matrix basis into groups based on shared matrix entries. For the most part, these subsets include measurements from both the W and W'. These are the fundamental measurement subsets to consider, not the W and W' subgroups we have imposed. There are four subsets of pauli matrices since each pauli matrix includes 4 entries, and our witnesses have 16 entries. We enumerate them here. The relations between and within subsets determine which witnesses are allowed.

4.3.3 Pauli Matrix Subset 0

The first group, after taking the partial transpose, contains $\sigma_0 \otimes \sigma_0$, $\sigma_z \otimes \sigma_0$, $\sigma_0 \otimes \sigma_z$, $\sigma_z \otimes \sigma_z$. This group is not very interesting - all the measurements it includes are only required for W. All of these entries are on the diagonal and are real - the only variance between elements in this subgroup is up to the negative signs on pairs of entries. What is important to note is that amongst this set of 4 measurements to take in the course of our witnessing procedure, taking the partial transpose of any of these matrices results in the same matrix. No additional measurements needed.

4.3.4 Pauli Matrix Subset 1

More interesting is the next subgroup, containing $\sigma_0 \otimes \sigma_x$, $\sigma_0 \otimes \sigma_y$, $\sigma_z \otimes \sigma_x$, $\sigma_z \otimes \sigma_y$. We can also note the entries required for these matrices are described by adding terms $|HH\rangle \langle HV|$, $|HV\rangle \langle HH|$, $|VH\rangle \langle VV|$,and $|VV\rangle \langle VH|$, with different real and imaginary contributions from each of those entries. The matrices are given in equation 4.3 below:

$$\sigma_0 \otimes \sigma_x = \begin{bmatrix} . & 1 & . & . \\ 1 & . & . & . \\ . & . & . & 1 \\ . & . & 1 & . \end{bmatrix} \quad \sigma_0 \otimes \sigma_y = \begin{bmatrix} . & i & . & . \\ -i & . & . & . \\ . & . & . & i \\ . & . & -i & . \end{bmatrix}$$
$$\sigma_z \otimes \sigma_x = \begin{bmatrix} . & 1 & . & . \\ 1 & . & . & . \\ . & . & . & -1 \\ . & . & -1 & . \end{bmatrix} \quad \sigma_z \otimes \sigma_y = \begin{bmatrix} . & i & . & . \\ -i & . & . & . \\ . & . & . & -i \\ . & . & i & . \end{bmatrix} \tag{4.3}$$

To look for patterns in our subset, we can factor the pauli matrix pairs into possible states for an outer product. We can get the desired matrix entries with the generic state $|\Psi\rangle = |HH\rangle + |HV\rangle + |VH\rangle + |VV\rangle$ upon $(|\Psi\rangle\langle\Psi|)^{\Gamma}$. We know that each ket must have some phase that produces the imaginary component, but only on some pauli measurements of that subset. Also, each of the matrices in the subset is distinct from the others.

From this, we realize that each measurement combination of our subset accrues a phase that results in a minus sign or imaginary component on a different ket relative to each of the other matrices in the subset. For example, consider the $\sigma_0 \otimes \sigma_y$ state and the $\sigma_z \otimes \sigma_y$ states. One possible state that produces the $\sigma_0 \otimes \sigma_y$ measurement is $|\Psi_{0y}\rangle = |HH\rangle + |VH\rangle + e^{i\pi/2}(|HV\rangle + |VV\rangle)$, whereas for $\sigma_z \otimes \sigma_y$ we have $|\Psi_{zy}\rangle = |HV\rangle + |VH\rangle + e^{i\pi/2}(|HH\rangle + |VV\rangle)$. Comparing these, each element of the subset has a state with relative phases on different components distinct from the others. As a result, the four generic states that produce our pauli matrices will all have shared components. However, they will all have different phases in the outer product cross-terms. This means they each accidentally include different pauli matrices.

4.3.5 Pauli Matrix Subset 2

We can repeat similar analysis for each of the next two subsets. The third subset contains $\sigma_x \otimes \sigma_0, \sigma_y \otimes \sigma_0, \sigma_x \otimes \sigma_z, \sigma_y \otimes \sigma_z$. The matrices all share common entries with different real and imaginary components of $|HH\rangle\langle VH|$, $|HV\rangle\langle VV|$, $|VH\rangle\langle HH|$,and $|VV\rangle\langle HV|$. These matrices are given in equation 4.4 below:

$$
\begin{aligned}
\sigma_x \otimes \sigma_0 &= \begin{bmatrix} . & . & 1 & . \\ . & . & . & 1 \\ 1 & . & . & . \\ . & 1 & . & . \end{bmatrix} \quad \sigma_y \otimes \sigma_0 = \begin{bmatrix} . & . & -i & . \\ . & . & . & -i \\ i & . & . & . \\ . & i & . & . \end{bmatrix} \\
\sigma_x \otimes \sigma_z &= \begin{bmatrix} . & . & 1 & . \\ . & . & . & -1 \\ 1 & . & . & . \\ . & -1 & . & . \end{bmatrix} \quad \sigma_y \otimes \sigma_z = \begin{bmatrix} . & . & -i & . \\ . & . & . & i \\ i & . & . & . \\ . & -i & . & . \end{bmatrix}
\end{aligned}
\tag{4.4}
$$

These matrices share the same properties as subsets 0 and 1, noting now that we have covered all the entries in the W'_{4-6} and W'_{7-9}. The measurements that go into W'_{4-6} and W'_{7-9} are notably in different subsets. In our overall goal to include some measurements and exclude others, we notice that the state we must outer product will result in cross-terms from other groups.

4.3.6 Pauli Matrix Subset 3

The last subgroup is the most interesting of all. It contains $\sigma_x \otimes \sigma_x, \sigma_y \otimes \sigma_y, \sigma_x \otimes \sigma_y, \sigma_y \otimes \sigma_x$ - all the additional measurements for W'_{1-3} beyond the W. This subgroup seems to be the odd one out because it includes a whole W' subgroup. It also includes imaginary terms only in the W' measurement components. It has matrix elements $|HH\rangle\langle VV|, |HV\rangle\langle VH|, |VH\rangle\langle HV|$, and $|VV\rangle\langle HH|$. The matrices are given below in equation 4.5:

$$
\begin{aligned}
\sigma_x \otimes \sigma_x &= \begin{bmatrix} . & . & . & 1 \\ . & . & 1 & . \\ . & 1 & . & . \\ 1 & . & . & . \end{bmatrix} \quad \sigma_y \otimes \sigma_y = \begin{bmatrix} . & . & . & 1 \\ . & . & -1 & . \\ . & -1 & . & . \\ 1 & . & . & . \end{bmatrix} \\
\sigma_x \otimes \sigma_y &= \begin{bmatrix} . & . & . & i \\ . & . & -i & . \\ . & i & . & . \\ -i & . & . & . \end{bmatrix} \quad \sigma_y \otimes \sigma_x = \begin{bmatrix} . & . & . & -i \\ . & . & -i & . \\ . & i & . & . \\ i & . & . & . \end{bmatrix}
\end{aligned}
\tag{4.5}
$$

4.3.7 Assessing New Witness Possibilities

The partial transpose of all of these matrices - in subsets 0 through 3 - is the same matrix, up to a negative sign. The entangled state density matrix that produces these pauli matrices must look very much like a state they would witness. An entangled state to be witnessed must also have a density matrix with similar elements to it's witness; the partial transpose stays within the same witness, and those do not require additional measurements. These subsets confirm our initial observations about the partial transpose and outer product in section 4.3.1.

Coming back to the original goal of this thesis, we wish to find a witness that has only $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_z$ to witness a state of the form $|\psi\rangle = \frac{1}{\sqrt{N}}(|HR\rangle + e^{i\theta}|RH\rangle)$. The partial transpose will not allow us to eliminate tricky cross-terms, or find some way out of including an additional measurement. If we want to find a witness that includes only $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_z$, the outer product of some entangled state must give it. What is more, $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_z$ are in the same pauli matrix subsets, with the same entry. This means that we are being even more exclusive than we initially thought. The full implications of the restrictions on our witness groupings are described in section 5.1.

Chapter 5

Mixing Subsets and New Witnesses

5.1 Mixing Subsets

The restrictions introduced in section 4.3 offer us some new insight. Now that we cannot simply expect to combine measurement subgroups randomly, we can meaningfully pick and choose which measurements we want to include in possible new witness sets. It is by following this path that we get two new types of witnesses: what we deem the V_1, V_2, V_3, and V_4, and W''_α, W''_β. We find that all other witnesses fall into a category 'compound witnesses' that require almost all the measurements for a full quantum tomography.

5.1.1 Witness Quadrants

Let us further explore the restrictions on a 4×4 witness by our pauli matrices. Some patterns start to emerge when we divide our witness into the subsets from section 4.3. We call these 'quadrants'. The phases and magnitudes of three 'quadrants' of our witness are restricted. Let us write our quadrants in a matrix, for visualization purposes. Subset 0 is along the diagonal, and remains unlabelled. Subset 1 has elements x, subset 2 has elements y, and subset 3 has elements z. Our matrix quadrants are displayed in the equation below, and reflect the matrix subsets we discussed in section 4.3.

$$\begin{bmatrix} . & x_1 & y_1 & z_1 \\ x_4 & . & z_3 & y_2 \\ y_4 & z_4 & . & x_3 \\ z_2 & y_3 & x_2 & . \end{bmatrix} \tag{5.1}$$

Both our density matrices and our witnesses are hermitian, so the upper triangle completely determines the lower triangle. Notice that each quadrants' entries can change with respect to one another with contributions from the pauli matrices included in W, within their own subsets. Then all the pauli matrix subsets can have different relative real magnitudes internally and externally. The same is true for the imaginary parts. This means we need to consider each pair of entries separately: how the pairs within a quadrant relate to each other determines which pauli matrices are included in our witness. For example, in subset 1, $\sigma_0 \otimes \sigma_y$ is only in the W, but $\sigma_z \otimes \sigma_y$ is in a W'. They both control $Im(x_1)$ and $Im(x_3)$, but with different phases. If our witness has overall unequal magnitudes of imaginary parts in entries x_1 and x_3, then it must contain both measurements. If it has equal magnitude imaginary parts, we know that it only contains one of the two bases measurements, and the phase difference between pairs of entries tells us which basis measurement.

5.1.2 Compound Witnesses

We may now consider what happens when we change relative properties within the quadrants in the same witness. First, let us begin by asking what happens when we change the magnitude or phase of one pair in a quadrant irrespective of the other. Pairs within quadrants of our witness with different phases and amplitudes may cause some problems. Consider for example, $|\psi\rangle = a\,|HH\rangle - bi\,|HV\rangle + ci\,|VH\rangle + di\,|VV\rangle$. In this case, we get the density matrix:

$$\begin{bmatrix} a^2 & abi & -aci & -adi \\ -abi & b^2 & -bc & -bd \\ aci & bc & c^2 & cd \\ adi & bc & cd & d^2 \end{bmatrix} \tag{5.2}$$

We can see that the quadrants have different sets of pairs: one with imaginary entries, and the other with real entries. This means that we need to sum both the imaginary matrices in each subset, and both real matrices to describe the witness. In short, each quadrant has all matrices from that subset. In this example, we include $\sigma_0 \otimes \sigma_y$, $\sigma_z \otimes \sigma_y$, $\sigma_0 \otimes \sigma_x$, $\sigma_z \otimes \sigma_x$, $\sigma_y \otimes \sigma_z$, $\sigma_y \otimes \sigma_0$, $\sigma_x \otimes \sigma_z$, $\sigma_x \otimes \sigma_0$, $\sigma_x \otimes \sigma_y$, $\sigma_y \otimes \sigma_y$, $\sigma_y \otimes \sigma_x$, and $\sigma_x \otimes \sigma_x$. Too many additional measurements to have a useful witness! We call these the 'compound witnesses' because they require adding different pauli matrices to account for pair discrepancies in each quadrant. To get a witness that requires W measurements and not much else, the whole quadrant must have pairs that belong to the same pauli matrix subset, where the pairs are both imaginary or both real. Having mixes of the way pairs interact produces compound witnesses; if we do not consider the phases of our pairs, we may end up with a witness that contains too many measurements.

5.1.3 No New Two-Measurement Witnesses

Next, we can investigate the possible new witnesses produced by this quadrant-driven formulation. Let us return to our initial goal: find new witnesses with two measurements in the second step of the two step process, one from each W' group. In order to achieve this goal, we would need to have either one single measurement from two different pauli matrix subsets, or two measurements from the same pauli matrix subset. This will allow us to get a measurement from two different W' subgroups.

Having two W' measurements from the same subset combines a real and imaginary matrix from each W' group, excluding the case of subset 3. Since both components are in the same subset, we include some real or imaginary component in another quadrant. Our witness must be decomposable, so we would require cross-terms in at least one other quadrant that have an additional imaginary component, or have imaginary components that become real. The fourth subset doesn't follow this rule because both the imaginary matrices included are in W'_{7-9}.

Otherwise, if we include measurements from different W' and different subsets, we must have one quadrant of our witness have imaginary components, and the other real components. W' subgroups additional measurement pauli matrices are either all imaginary or all real. To sample from both W'_{1-3} and W'_{4-6}, we sample one real pauli matrix pair and one imaginary pauli matrix pair. This leaves either a single compound quadrant, or one quadrant with imaginary components and one with real. When we choose the latter, we would have a state to outer product with two imaginary terms. For example, consider:

$$|\psi\rangle = \frac{1}{2}(|HH\rangle - i\,|HV\rangle + |VH\rangle + i\,|VV\rangle)$$

This state would sample from two W' measurement groups, but would produce imaginary diagonal entries $|HH\rangle\langle VV|$ and $|VV\rangle\langle HH|$, and therefore accidentally includes an extra W' subgroup in the cross terms. The fourth subset provides an additional challenge. We can have only one measurement from W'_{7-9} if we are sampling different subsets, but since those are anti-diagonal terms, they must also have cross-terms that are imaginary in some other quadrant, leaving the other real and with an extra phase accrued.

Enumerating all the cases, this means we cannot have only two measurements pulled from different W'. We always somehow implicate a third measurement, or more. These third measurements lead to two new types of witness groups.

5.1.4 Changes to the Two-Step Process

The new witness groups, which we choose to call V_1, V_2, V_3, V_4, and W''_α, W''_β, are now easy to define based on our generic matrix formalism of our witness state. The new witness subgroups offer two alternative ways to improve upon the two-step process. The V_1, V_2, V_3, V_4 (named as an alternative to the W') have three measurements instead of two, one from each W', one from each subgroup. These would be an alternative to W's in the two-step process. Additionally, the W''_α, W''_β improve upon the existent process. They contain three measurements: two from one W' group, and one additional measurement from another W' group. In terms of the subsets defined in section 4.1, they sample from two different pauli subsets to obtain the W' measurements, and then sample one additional measurement from one of the pauli subsets already considered. Tables 5.1, 5.2, 5.3, 5.4 show the measurements for the $\{V\}$ witnesses. Tables 5.5 and 5.6 show the measurements for the $\{W''\}$ witnesses

5.2 The New $\{V\}$ Witnesses

We define the new set of witnesses $\{V\}$ as witnesses that contain three pauli basis measurement pairs, each from different W' subgroups. All of these witnesses require measurements like $\sigma_i \otimes \sigma_j$, $\sigma_j \otimes \sigma_k$, $\sigma_i \otimes \sigma_k$, where we get a different V_i for different ordering of i, j, k. The witnesses V_1, V_2, V_3 and V_4 are defined by which pauli basis measurements we choose to include and exclude while still fitting this form. Containing some pauli-matrix pairs produces additional constraints that allow us to parameterize our witness. Using the generic witness we defined in section 5.1, we can now significantly decrease the number of parameters required for our witnesses. For our generic witness, let a, b, c, d all be real numbers such that $a^2 + b^2 + c^2 + d^2 = 1$ to obey normalization constraints. This allows us to specify all properties of our witness quadrants with phases.

5.2.1 The V_1 Witnesses

$\sigma_x \otimes \sigma_x$	$\sigma_x \otimes \sigma_y$	$\sigma_x \otimes \sigma_z$
$\sigma_y \otimes \sigma_x$	$\sigma_y \otimes \sigma_y$	$\sigma_y \otimes \sigma_z$
$\sigma_z \otimes \sigma_x$	$\sigma_z \otimes \sigma_y$	$\sigma_z \otimes \sigma_z$

Table 5.1 V_1 subgroup measurements from full quantum tomography. $\sigma_z \otimes \sigma_y, \sigma_x \otimes \sigma_z, \sigma_x \otimes \sigma_y$ are required. The light blue colored entries indicate measurements that are required for the original W subgroup. The pink cells show the measurements that are included in V_1, and the grey cells show the measurements that are excluded.

The V_1 constraints require us to revisit the pauli matrix subset defined in section 5.1. These witnesses contain $\sigma_z \otimes \sigma_y$, $\sigma_x \otimes \sigma_z$, $\sigma_x \otimes \sigma_y$, and exclude other pauli measurements beyond the W measurements. To contain $\sigma_z \otimes \sigma_y$ but not $\sigma_z \otimes \sigma_x$, we must have that the imaginary components in the x_1, x_3 not match, such that $Im(x_1) \neq Im(x_3)$. We do not strictly require $-Im(x_1) = Im(x_3)$ because the other pauli matrix pair in the first subset is $\sigma_0 \otimes \sigma_y$, and is included in the W measurements. Therefore, in a possible V_1, it can be a component. This means that we may have unequal imaginary parts within our quadrant: our possible witnesses need not obey strict phase conditions. Excluding $\sigma_z \otimes \sigma_x$ from the quadrant, following similar logic to the pairings of $\sigma_z \otimes \sigma_y$ and $\sigma_0 \otimes \sigma_y$, $\sigma_0 \otimes \sigma_x$ is a natural pair. It contributes to the real part of these entries without requiring extra measurements. Therefore, we only want matrices with $\sigma_0 \otimes \sigma_x$ for the real part. This gives that $Re(x_1) = Re(x_3)$. We may follow the same process for the second quadrant. Here, we wish to include $\sigma_x \otimes \sigma_z$, and exclude $\sigma_y \otimes \sigma_z$. This gives us the constraints that $Re(y_1) \neq Re(y_2)$, and that $Im(y_1) = Im(y_2)$. For the third quadrant, we must choose either a $\sigma_x \otimes \sigma_y$ or a $\sigma_y \otimes \sigma_x$. First choosing $\sigma_x \otimes \sigma_y$, we get that $-Im(z_1) \neq Im(z_3)$.

Altogether, these constraints result in the following values of our parameterized witness. Much like in our parameterized witness, we must have that $a^2 + b^2 + c^2 + d^2 = 1$ where all are real. Solving for b, c and d given our limitations, we get the solutions described in equation 5.5:

$$b = a\sqrt{\frac{\sin(\gamma)\sin(\delta)}{\sin(\gamma-\beta)\sin(\beta-\delta)}} \tag{5.3}$$

$$c = a\sqrt{\frac{-\cos(\beta)\sin(\delta)}{\cos(\gamma-\delta)\sin(\gamma-\beta)}} \tag{5.4}$$

$$d = a\sqrt{\frac{-\cos(\beta)\sin(\gamma)}{\cos(\gamma-\delta)\sin(\beta-\delta)}} \tag{5.5}$$

Substituting these parameters into our generic parameterized witness in equation 4.1, we get the class of witnesses called the V_1 witnesses. The measurements for the V_1 witnesses are shown in table 5.1.

5.2.2 The V_2 Witnesses

$\sigma_x \otimes \sigma_x$	$\sigma_x \otimes \sigma_y$	$\sigma_x \otimes \sigma_z$
$\sigma_y \otimes \sigma_x$	$\sigma_y \otimes \sigma_y$	$\sigma_y \otimes \sigma_z$
$\sigma_z \otimes \sigma_x$	$\sigma_z \otimes \sigma_y$	$\sigma_z \otimes \sigma_z$

Table 5.2 V_2 subgroup measurements from full quantum tomography. $\sigma_z \otimes \sigma_y$, $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_x$ are required. The light blue colored entries indicate measurements that are required for the original W subgroup. The pink cells show the measurements that are included in V_2, and the grey cells show the measurements that are excluded.

With similar constraints on a, b, c, and d, we get the next class of witnesses, V_2. These include $\sigma_z \otimes \sigma_y$, $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_x$. The logic is identical to V_1 for the first two quadrants of the witness. For the third, we now must include $\sigma_y \otimes \sigma_x$ and exclude $\sigma_x \otimes \sigma_y$. To do this, we must now require that $Im(z_1) \neq Im(z_3)$, and instead that $-Im(z_1) = Im(z_3)$. Note again that we must have $a^2 + b^2 + c^2 + d^2 = 1$ where all are real. These conditions allow us to solve for b, c and d displayed in 5.8 below.

$$b = a\sqrt{\frac{-\sin(\gamma)\sin(\delta)}{\sin(\gamma-\beta)\sin(\beta-\delta)}} \tag{5.6}$$

$$c = a\sqrt{\frac{\cos(\beta)\sin(\delta)}{\cos(\gamma-\delta)\sin(\gamma-\beta)}} \tag{5.7}$$

$$d = a\sqrt{\frac{-\cos(\beta)\sin(\gamma)}{\cos(\gamma-\delta)\sin(\beta-\delta)}} \tag{5.8}$$

Again, these values can be substituted into equation 4.1 to get the witness class V_2. The measurements for the V_2 witnesses are shown in table 5.2.

5.2.3 The V_3 Witnesses

$\sigma_x \otimes \sigma_x$	$\sigma_x \otimes \sigma_y$	$\sigma_x \otimes \sigma_z$
$\sigma_y \otimes \sigma_x$	$\sigma_y \otimes \sigma_y$	$\sigma_y \otimes \sigma_z$
$\sigma_z \otimes \sigma_x$	$\sigma_z \otimes \sigma_y$	$\sigma_z \otimes \sigma_z$

Table 5.3 V_3 subgroup measurements from full quantum tomography. $\sigma_z \otimes \sigma_x$, $\sigma_y \otimes \sigma_z$ and $\sigma_x \otimes \sigma_y$ are required. The light blue colored entries indicate measurements that are required for the original W subgroup. The pink cells show the measurements that are included in V_3, and the grey cells show the measurements that are excluded.

We can now impose constraints on a, b, c and d to get the next class of witnesses, V_3. These include $\sigma_z \otimes \sigma_x$, $\sigma_y \otimes \sigma_z$ and $\sigma_x \otimes \sigma_y$. Now we have for quadrant 1 that $Re(x_1) \neq Re(x_3)$ but that $-Im(x_1) = Im(x_3)$. For the second quadrant, we get that $Re(y_1) = Re(y_2)$ and $-Im(y_1) \neq Im(y_2)$. For the third, we now must exclude $\sigma_y \otimes \sigma_x$ and include $\sigma_x \otimes \sigma_y$. To do this, we require that $Im(z_1) = Im(z_3)$, and that $-Im(z_1) \neq Im(z_3)$. Note again that we must have $a^2 + b^2 + c^2 + d^2 = 1$ where all are real. These conditions allow us to solve for b, c and d displayed in 5.11 below.

$$b = a\sqrt{\frac{-\cos(\gamma)\sin(\delta)}{\sin(\gamma-\beta)\cos(\beta-\delta)}} \tag{5.9}$$

$$c = a\sqrt{\frac{\sin(\beta)\sin(\delta)}{\sin(\gamma-\delta)\sin(\gamma-\beta)}} \tag{5.10}$$

$$d = -a\sqrt{\frac{-\sin(\beta)\cos(\gamma)}{\sin(\gamma-\delta)\cos(\beta-\delta)}} \tag{5.11}$$

These values can be substituted into equation 4.1 to get the witness class V_3. The measurements for the V_3 witnesses are shown in table 5.3.

5.2.4 The V_4 Witnesses

$\sigma_x \otimes \sigma_x$	$\sigma_x \otimes \sigma_y$	$\sigma_x \otimes \sigma_z$
$\sigma_y \otimes \sigma_x$	$\sigma_y \otimes \sigma_y$	$\sigma_y \otimes \sigma_z$
$\sigma_z \otimes \sigma_x$	$\sigma_z \otimes \sigma_y$	$\sigma_z \otimes \sigma_z$

Table 5.4 V_3 subgroup measurements from full quantum tomography. $\sigma_z \otimes \sigma_x$, $\sigma_y \otimes \sigma_z$ and $\sigma_y \otimes \sigma_x$ are required. The light blue colored entries indicate measurements that are required for the original W subgroup. The pink cells show the measurements that are included in V_4, and the grey cells show the measurements that are excluded.

For the final witness class of the $\{V\}$ set, we again impose a set of constraints based on including some basis measurements and excluding others. The V_4 include $\sigma_z \otimes \sigma_x$, $\sigma_y \otimes \sigma_z$ and $\sigma_y \otimes \sigma_x$. We have for quadrant 1 that $Re(x_1) \neq Re(x_3)$ and that $-Im(x_1) = Im(x_3)$. For the second quadrant, we get that $Re(y_1) = Re(y_2)$ and $-Im(y_1) \neq Im(y_2)$. For the third, we now must include $\sigma_y \otimes \sigma_x$ and exclude $\sigma_x \otimes \sigma_y$. To do this, we require that $Im(z_1) \neq Im(z_3)$, and that $-Im(z_1) = Im(z_3)$. Note again that we must have $a^2 + b^2 + c^2 + d^2 = 1$ where all are real. These conditions allow us to solve for b, c and d displayed in 5.14 below.

$$b = a\sqrt{\frac{\cos(\gamma)\sin(\delta)}{\sin(\gamma-\beta)\cos(\beta-\delta)}} \tag{5.12}$$

$$c = a\sqrt{\frac{-\sin(\beta)\sin(\delta)}{\sin(\gamma-\delta)\sin(\gamma-\beta)}} \tag{5.13}$$

$$d = -a\sqrt{\frac{-\sin(\beta)\cos(\gamma)}{\sin(\gamma-\delta)\cos(\beta-\delta)}} \tag{5.14}$$

These values can be substituted into equation 4.1 to get the witness class V_4. This is the final witness class in the $\{V\}$. The measurements for the V_4 witnesses are shown in table 5.4.

5.3 W''_α and W''_β

We can next consider the set of witnesses produced by adding an additional measurement to the W' group. This would happen in a 'third step' of the two-step process: after picking a W' subgroup, we could pick an additional useful measurement. We have two witness considerations: witnesses that have W'_{7-9} and only one measurement from W'_{4-6}, or a witness with W'_{4-6} and only one measurement from W'_{7-9}. These produces the W''_α, which have $\sigma_x \otimes \sigma_z$, $\sigma_z \otimes \sigma_x$, and $\sigma_y \otimes \sigma_z$ and the W''_β, which have $\sigma_y \otimes \sigma_z$, $\sigma_z \otimes \sigma_y$, and $\sigma_x \otimes \sigma_z$.

We cannot add to the W'_{1-3} group, because those measurements would require both of our imaginary contributions to be in the same quadrature. Since this quadrature also happens to be the anti-diagonal of the witness, we necessarily implicate cross terms and create a compound witness. For example, to create a witness with W'_{1-3}, we could use the state: $|\psi\rangle = |HH\rangle + e^{i\varphi}|HV\rangle + i|VH\rangle + i|VV\rangle$ with the extra phase added to include different possible W' pauli pairs. Because of the imaginary terms, $|\psi\rangle\langle\psi|$ would either create a W' group, or, if $\varphi \neq 0, \pi$, a compound witness. When $\varphi = \pi/2$, we get a witness from $\{V\}$. In any case, this $|\psi\rangle$ does not add to the set of W''.

5.3.1 The W''_α Witnesses

The W''_α group of witnesses has the witnesses described below, in table 5.15. By following the same logic as we used to define the $\{V\}$, we get constraints

$\sigma_x \otimes \sigma_x$	$\sigma_x \otimes \sigma_y$	$\sigma_x \otimes \sigma_z$
$\sigma_y \otimes \sigma_x$	$\sigma_y \otimes \sigma_y$	$\sigma_y \otimes \sigma_z$
$\sigma_z \otimes \sigma_x$	$\sigma_z \otimes \sigma_y$	$\sigma_z \otimes \sigma_z$

Table 5.5 W''_α subgroup measurements from full quantum tomography. $\sigma_z \otimes \sigma_x$, $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_z$ are required. The light blue colored entries indicate measurements that are required for the original W subgroup. The pink cells show the measurements that are included in W''_α, and the grey cells show the measurements that are excluded.

on our parameterization. By including $\sigma_z \otimes \sigma_x$, $\sigma_x \otimes \sigma_z$ and $\sigma_y \otimes \sigma_z$, but not $\sigma_z \otimes \sigma_y$, $\sigma_x \otimes \sigma_y$ and $\sigma_y \otimes \sigma_x$, we conditions, similar to the $\{V\}$. Since our anti-diagonal must be real to exclude the $\sigma_x \otimes \sigma_y$ and $\sigma_y \otimes \sigma_x$, we get limits on d and specific possible cases of δ, γ and β. To maintain the real diagonal, $\delta = 0, \pi$ and $\gamma = \beta + \pi$. Rather than enumerate the conditions as we did in section 5.2, these constraints let us compactly write the possible witnesses from equation 4.1. From this, we get the four cases. The four cases collapse to 2 when we realize the d and δ conditions counteract each other - by definition, d always comes with a δ. Then when d is negative and δ is π, we get the same result as if d were positive and $\delta = 0$. Again remember that we must have $a^2 + b^2 + c^2 + d^2 = 1$ where all are real. This leaves two cases, displayed in equation 5.15.

$$\begin{array}{ll|l} \delta = 0, \gamma = \beta, & d = \frac{-ab}{c} & \begin{bmatrix} a^2 & abe^{-i\beta} & ace^{-i\beta} & \frac{-a^2b}{c} \\ abe^{i\beta} & b^2 & bc & \frac{-ab^2}{c}e^{i\beta} \\ ace^{i\beta} & bc & c^2 & -abe^{i\beta} \\ \frac{-a^2b}{c} & \frac{-ab^2}{c}e^{-i\beta} & -abe^{-i\beta} & \frac{a^2b^2}{c^2} \end{bmatrix} \\ \delta = 0, \gamma = \pi + \beta, & d = \frac{ab}{c} & \begin{bmatrix} a^2 & abe^{-i\beta} & -ace^{-i\beta} & \frac{a^2b}{c} \\ abe^{i\beta} & b^2 & -bc & \frac{ab^2}{c}e^{i\beta} \\ -ace^{i\beta} & -bc & c^2 & -abe^{i\beta} \\ \frac{a^2b}{c} & \frac{ab^2}{c}e^{-i\beta} & -abe^{-i\beta} & \frac{a^2b^2}{c^2} \end{bmatrix} \end{array} \tag{5.15}$$

The measurements required for the W''_α are also shown in table 5.5.

5.3.2 The W''_β Witnesses

We define the W''_β to include the pauli matrix pairs $\sigma_z \otimes \sigma_y$, $\sigma_y \otimes \sigma_z$, and $\sigma_x \otimes \sigma_z$, excluding all other W' component measurements. Since our anti-

$\sigma_x \otimes \sigma_x$	$\sigma_x \otimes \sigma_y$	$\sigma_x \otimes \sigma_z$
$\sigma_y \otimes \sigma_x$	$\sigma_y \otimes \sigma_y$	$\sigma_y \otimes \sigma_z$
$\sigma_z \otimes \sigma_x$	$\sigma_z \otimes \sigma_y$	$\sigma_z \otimes \sigma_z$

Table 5.6 W''_β subgroup measurements from full quantum tomography. $\sigma_z \otimes \sigma_y$, $\sigma_y \otimes \sigma_z$ and $\sigma_x \otimes \sigma_z$ are required. The light blue colored entries indicate measurements that are required for the original W subgroup. The pink cells show the measurements that are included in W''_β, and the grey cells show the measurements that are excluded.

diagonal must be real, we again get the restriction $\delta = 0, \pi$ and $\gamma = 0, \beta + \pi$. Again remember that we must have $a^2 + b^2 + c^2 + d^2 = 1$ where all are real. From these restrictions, we also get additional constraints on d. Since d is always paired with a δ, if d is negative and $\delta = \pi$ we get the same conditions as if d were positive and $\delta = 0$. This collapses our four cases into two, and one of those cases is covered by the W''_α. The resulting witnesses are in equation 5.16.

$$\delta = 0, \gamma = \beta, \quad d = \frac{ab}{c} \left| \begin{bmatrix} a^2 & abe^{-i\beta} & ace^{-i\beta} & \frac{a^2b}{c} \\ abe^{i\beta} & b^2 & bc & \frac{ab^2}{c}e^{i\beta} \\ ace^{i\beta} & bc & c^2 & abe^{i\beta} \\ \frac{a^2b}{c} & \frac{ab^2}{c}e^{-i\beta} & abe^{-i\beta} & \frac{a^2b^2}{c^2} \end{bmatrix} \right. \tag{5.16}$$

The measurements required for the W''_β are also shown in table 5.6.

These new subsets of witnesses may offer an alternative to the current W' role in the two-step process, or may add on to the two-step process. The full implications of this are discussed in the next chapter.

5.4 New Witnesses: Promising Initial Characterization

This range of new possible witnesses is certainly promising. The next step is to determine whether these new witnesses see any new states that are missed by the W and W'. We run brief characterization simulations of a candidate from the $\{W''\}$, and multiple candidates from the $\{V\}$ sets. Using the Roik et al. (2021) method randomly generated states from the Quantum Optic's group Scholin et al. (2023), we find the expectation values of all the witness groups - the $\{W\}$, $\{W'_{1-3}\}$, $\{W'_{4-6}\}$, $\{W'_{7-9}\}$, V, W'' - and return whether or not a group witnessed each state. We compare which states each subset witnessed to find whether the states witnessed overlap between groups. We find that both the V and W'' candidates witness states that are missed by all other witness groups. The W, W' groups are minimized, while the V and W'' candidates are not. The V and W'' minimization has yet to be implemented.

5.4.1 The V Witness Characterization

The V witnesses picked for the simulation are equal magnitude representatives of each of the possible V subsets. The states for these are:

$$\begin{aligned}
|\phi_1\rangle &= \frac{1}{2}(|HH\rangle + |HV\rangle - i\,|VH\rangle + i\,|VV\rangle)\\
|\phi_2\rangle &= \frac{1}{2}(|HH\rangle - |HV\rangle + i\,|VH\rangle + i\,|VV\rangle)\\
|\phi_3\rangle &= \frac{1}{2}(|HH\rangle - i\,|HV\rangle - |VH\rangle - i\,|VV\rangle)\\
|\phi_4\rangle &= \frac{1}{2}(|HH\rangle + i\,|HV\rangle - |VH\rangle + i\,|VV\rangle)
\end{aligned}$$

Where each state forms a witnesses such that $|\phi_1\rangle$ is from V_1, $|\phi_2\rangle$ is from V_2, $|\phi_3\rangle$ is from V_3, and $|\phi_4\rangle$ is from V_4. For each, $|\phi_i\rangle\langle\phi_i|^\Gamma$ is the representative witness. With these, and four other witnesses such that there are two representing every subset, we checked the efficiency and overlap of the states.

Combining all V witnesses, without any optimization, the V set witnessed 4.8% of the possible randomly generated entangled states. Of all the randomly generated entangled states, 0.35% of states that were witnessed by the V went unwitnessed by any of the W or W'.

Even without optimization, the V witnesses contribute new states that have been unwitnessed by the two-step process so far. Though the number of states is small, with optimization, it is possible that the number will increase significantly, along with the efficiency. Since only 20% of states remain unwitnessed by the two-step process, even a few percent total by the V witnesses can make them advantageous.

5.4.2 The W'' Witness Characterization

Much like the V witnesses, the W'' hold promising results. The W'' witness representative is a witness from W''_{β}. This witness has a state:

$$|\psi\rangle = 2\,|HH\rangle + 2e^{i\frac{\pi}{4}}\,|HV\rangle + e^{i\frac{\pi}{4}}\,|VH\rangle + |VV\rangle$$

We can take the outer product and partial transpose of this state to get the corresponding witness. This witness is also not optimized. Without optimization, it witnesses 3.3% of the randomly generated entangled states. The class of these witnesses see 0.01% of states that are missed by the W and W'. Upon optimization, this number may increase. The random witness picked is almost certainly not the best witness for each of the possible states. As such, minimization of the W'' and V are the next step to determine how effective these witness groups really are in comparison to the W and W'.

5.4.3 More Improvement Alternatives

If upon minimization both the $\{V\}$ and $\{W''\}$ witnesses are not useful additions to the two-step process, we could return to the tried-and-true W'. Picking a W', then adding another step to the two-step process to pick another W', could witness more states. The W' currently leave 27.7% of states undetected when using the 5-layer neural network picking mechanism. Though we may come closer to doing a full tomography, two extra measurements could witness a significant number of missed states. Since the W' are already very effective, the new combinations of pauli measurements we create when we combine W' may be very effective.

5.5 Summary

This chapter has discussed the wide range of possible decomposable witness subgroups. We detail the existing W' subgroups, and the motivation for moving beyond them. We introduce a parameterized generic entanglement witness. We then introduce subsets of pauli basis pairs based on shared entries of the pauli basis matrices. These four subcategories, deemed subsets 0, 1, 2, and 3 provide a basis to demonstrate how the partial transpose of a witness measurement is closed on the same matrix, requiring all the same measurements of a witness as a state. The outer product, however, can cause problematic cross-terms that prevent two-matrix witnesses beyond the W'.

We show the limitations these new subsets place on our witnessing structure (i.e. we cannot pick and choose witness measurements arbitrarily). Finally, we introduce the new witness sets, the V, W'' that offer alternatives to the current two-step process. We share the preliminary characterization results, and find that these witnesses do witness states that are missed by prior witnessing protocols.

Chapter 6

Next Steps

After the introduction of the $\{V\}$ and $\{W''\}$, there are many possible amendments to the two-step process. One improvement need not be better than another: they may be implemented concurrently. The best way to determine which methods are best to implement next is by first assessing the performance of new witnesses. This chapter focuses on assessing the new witness subgroups as possible ways to update the current two-step process. We also advise new ways to parameterize entanglement witnesses.

6.1 Next Steps: Minimization

The most pressing course of action for characterizing the $\{V\}$ and $\{W''\}$ is to determine how many states they witness. And more importantly, how effective they are compared to W'. This can be done by minimizing the $\{V\}$ and $\{W''\}$ free parameters for each entangled state in a set of randomly generated entangled states. We can then determine how many of those random states the $\{V\}$ and $\{W''\}$ witness.

6.2 Assessing Witness Subgroups

The $\{V\}$ and $\{W''\}$ offer different alternatives to the current entanglement witnessing procedure. The $\{V\}$ witness groups represent an alternative to W'. Rather than allow a neural network to pick from different sets of W', there are more possibilities. Witness subgroups generated by W', V_1, V_2, V_3, V_4 may all be thrown into the mix, and the neural network should be able to pick between those subgroups. However, it should be taken into account that the W' have fewer measurements than the $\{V\}$. In addition to current neural network picking technique, the neural network should be amended to consider the number of measurements and not pick from the $\{V\}$ witnesses in the case that they are not more efficient.

For the $\{W''\}$ subgroups, more needs to be done. In the case the W'' are picked, there are multiple possibilities for next steps. There can be two neural networks (or similar picking mechanisms) to create a three-step process. In this case, given the neural network in the first step picked W'_{1-3} or W'_{4-6} and the state was missed, the second neural network could pick a W''. This would allow multiple exit points: at each picking stage, if the state of interest was witnessed, no additional measurements need be taken. Alternately, much like the $\{V\}$, it is possible to simply allow one neural network to pick from a wider array of witness possibilities in the first stage of the two-step process.

No matter the picking mechanism, the $\{V\}$ and $\{W''\}$ do add to the states measurable by the two-step process. The $\{V\}$ and $\{W''\}$ all witness states that are unwitnessed by W and W' witnesses. How many states they witness, and how efficient they are independent of the W', has yet to be determined.

6.3 Next Steps: Generalization

The other pressing concern for the new witness subgroups is generalization. Defining a new set of witness subgroups illuminated that we do not have an algebraically concise way to parameterize witnesses. Based on the subsets we found in this thesis, we believe it is possible to treat the pauli basis subsets as generators of witness sets. The witness subgroups outlined in section 4.3 suggests that there is a way to parameterize witnesses more efficiently, and to set a firm mathematical bound on which witnesses are possible.

One way to go about this is by considering each of the subsets outlined above as a generator of a group of witnesses, and formalize this subgroup. Still, the large number of parameters in the final witnesses generated by such a subgroup indicates that there may possibly be some degeneracy in this approach. It also does not illuminate why certain witnesses are possible, and others are not.

Another approach is by considering the entanglement witness as a density matrix representation of some entangled state. In this case, there are multiple formalisms that allow parameterization of a generic entangled state. Maybe, by considering a different parameterization, it will be possible to gain new insights about why specific witness subgroups emerge.

Chapter 7

Conclusion

7.1 Conclusions

We have found two new classes of entanglement witnesses, yet to be fully characterized. These witnesses can either compliment or replace the existing two-stage entanglement detection protocol that the we employ.

Our new entanglement witnesses witness randomly generated states that are missed by our two-stage entanglement detection protocol. However, they must be minimized, integrated into the existing protocol, and fully generalized. Upon creating these new classes of witnesses, we also impose restrictions on the existence of some witnesses. These restrictions are fundamentally tied to the witness structure under some parameterization, and have yet to be mathematically formalized.

Future investigation into the effectiveness of the proposed witnesses and into parameterizing the witnesses mathematically is needed to explore the full range of these new witness groups. Happy witness hunting.

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