

Gate Fidelity Fluctuations and Quantum Process Invariants

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Abstract

We characterize the quantum gate fidelity in a state-independent manner by giving explicit expressions for the variance and a method for calculating all moments of the gate fidelity. Using these results we discuss a method for determining the time evolution of the variance of the gate fidelity in the case of Markovian noise. We analyze the limiting cases of a single qubit and large-dimensional quantum systems. Applications of these results to quantum chaos and randomized benchmarking are also discussed.

1 Introduction

In quantum information science, quantum systems are transformed by applying unitary operations or *gates*. Real experimental implementations of a gate are always imprecise: we wish to apply the gate \mathcal{U} , but instead we apply some quantum operation \mathcal{E} . One useful measure of how close \mathcal{U} and \mathcal{E} are is the *gate fidelity* $\mathcal{F}_{\mathcal{E},\mathcal{U}}$ (a.k.a channel fidelity) between \mathcal{U} and \mathcal{E} . The gate fidelity between \mathcal{E} and \mathcal{U} is the function on quantum states with action given by,

$$\mathcal{F}_{\mathcal{E},\mathcal{U}}(\rho) = \left(\text{tr} \sqrt{\sqrt{\mathcal{E}(\rho)} \mathcal{U}(\rho) \sqrt{\mathcal{E}(\rho)}} \right)^2.$$

Here ρ is a quantum state and the right hand side is the familiar *state fidelity* between $\mathcal{E}(\rho)$ and $\mathcal{U}(\rho)$.

The goal of this paper is to remove the dependence on the input state by calculating state-independent properties of the gate fidelity – specifically, its mean and variance over the uniform distribution on pure input states. The first order information for how much the quantum operation deviates from the unitary is given by the mean of the gate fidelity [13, 7]. Knowledge of higher order moments for the gate fidelity allows for the determination of the shape of the gate fidelity around its average.

One expression for the variance of the gate fidelity between a unitary operator and a linear operator mapping into pure states has been given in [15]. In this paper we relax the unnecessary restriction to linear operators mapping into pure states and consider a general quantum operation with range given by all quantum states. In addition, the method we use to obtain the variance is new and extends to calculate all higher order moments. We also obtain various equivalent expressions for the variance in terms of invariants of the quantum process. Our calculation also allows for

an analysis of specific cases, examples of which are the single qubit case and the case of large dimensional quantum systems.

The paper is laid out as follows: The first section deals with the background required for the rest of the paper. Since the method we use for calculating the variance can be used to calculate all moments we use it to calculate the average fidelity in the next section and show that the result is consistent with known expressions.

Next, the variance is calculated in terms of both the Kraus and χ -matrix [5] representations and calculating higher order moments is discussed. In the following section we use the expression for the variance in terms of the χ -matrix to obtain an expression in terms of the Choi-Jamiolkowski state. One advantage for this representation is that it allows for a more simple method to determine the time evolution of the variance in the case of Markovian noise.

We use the χ -matrix and Choi-Jamiolkowski state representations of the variance to analyze two cases of interest, that of a single qubit and when the dimension of the quantum system grows large. Simple expressions for the variance are given for a single qubit, and for large dimensions the variance is shown to decrease as the inverse of the dimension.

We conclude with a discussion of our results. In particular we discuss the relevance of the results obtained to randomized protocols for noise characterization, and to estimating the fidelity decay under controlled perturbations in the context of simulating quantum chaotic systems with a quantum information processor.

2 Background

2.1 Gate Fidelity

Before beginning let us set some notation for the rest of the paper. Let \mathcal{H} represent the Hilbert space for a quantum system of dimension D and $\mathcal{D}(\mathcal{H})$ represent the set of states for the system. The set of pure states for a quantum system is represented by complex projective space $\mathbb{C}\mathbb{P}^{D-1}$. For any operator $A \in L(\mathcal{H})$ we define

$$[A] = \text{tr}(A) \tag{1}$$

which will make many of the following equations less cumbersome.

For $\rho, \sigma \in \mathcal{D}(\mathcal{H})$, the fidelity F between ρ and σ is defined by,

$$F(\rho, \sigma) = \left(\text{tr} \sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right)^2. \tag{2}$$

The fidelity is a useful measure of how far apart two states are in terms of deviation of measurement statistics. Realistically when one intends to apply a quantum gate, represented by a unitary operator \mathcal{U} , there is an error in the implementation. The imperfect operation is represented by some quantum operation \mathcal{E} . The gate-fidelity $\mathcal{F}_{\mathcal{E}, \mathcal{U}}$ is a useful state-dependent description of how close two quantum operations are. If $\rho \in \mathcal{D}(\mathcal{H})$ then $\mathcal{F}_{\mathcal{E}, \mathcal{U}}$ is defined as,

$$\mathcal{F}_{\mathcal{E}, \mathcal{U}}(\rho) := F(\mathcal{E}(\rho), \mathcal{U}(\rho)) = \left(\text{tr} \sqrt{\sqrt{\mathcal{E}(\rho)} \mathcal{U}(\rho) \sqrt{\mathcal{E}(\rho)}} \right)^2. \tag{3}$$

We are interested in the case when the input state is pure. If $\phi \mapsto |\phi\rangle\langle\phi| \in \mathbb{C}\mathbb{P}^{D-1}$ then,

$$\mathcal{F}_{\mathcal{E},\mathcal{U}}(\phi) = \text{tr}(\mathcal{U}(|\phi\rangle\langle\phi|)\mathcal{E}(|\phi\rangle\langle\phi|)). \quad (4)$$

If $\{M_k\}$ and U are Kraus operators for \mathcal{E} and \mathcal{U} respectively then using the cyclic property of the trace this can be rewritten as

$$\begin{aligned} \mathcal{F}_{\mathcal{E},\mathcal{U}}(\phi) &= \text{tr}\left(U|\phi\rangle\langle\phi|U^\dagger \sum_k M_k|\phi\rangle\langle\phi|M_k^\dagger\right) \\ &= \text{tr}(|\phi\rangle\langle\phi|\mathcal{U}^\dagger \circ \mathcal{E}(|\phi\rangle\langle\phi|)). \end{aligned} \quad (5)$$

Defining $\Lambda = \mathcal{U}^\dagger \circ \mathcal{E}$,

$$\mathcal{F}_{\mathcal{E},\mathcal{U}}(\phi) = \text{tr}(|\phi\rangle\langle\phi|\Lambda(|\phi\rangle\langle\phi|)) \quad (6)$$

where Λ represents how much \mathcal{E} deviates from \mathcal{U} .

There is a natural measure one can put on $\mathbb{C}\mathbb{P}^{D-1}$ called the Fubini-Study (FS) measure [2] which we will denote by μ_{FS} . μ_{FS} is the Borel measure induced by the Fubini-Study metric on $\mathbb{C}\mathbb{P}^{D-1}$, and is the unique unitarily invariant probability measure on $\mathbb{C}\mathbb{P}^{D-1}$. The average fidelity under the FS measure, $\overline{\mathcal{F}_{\mathcal{E},\mathcal{U}}} = \int_{\mathbb{C}\mathbb{P}^{D-1}} \mathcal{F}_{\mathcal{E},\mathcal{U}} d\mu_{FS}$, is given by

$$\begin{aligned} \overline{\mathcal{F}_{\mathcal{E},\mathcal{U}}} &= \int \text{tr}(|\psi\rangle\langle\psi|\Lambda(|\psi\rangle\langle\psi|)) d\psi \\ &= \frac{\sum_i (\text{tr}(K_i)\text{tr}(K_i^\dagger)) + D}{D^2 + D} \end{aligned} \quad (7)$$

where the $\{K_i\}$ are a set of Kraus operators for Λ [7, 13].

2.2 Generalized Gell-Mann Operators

There are various methods of generalizing the properties of the familiar Pauli operators on a single qubit to an arbitrary qudit. The generalization we will use throughout the rest of the discussion are the generalized Gell-Mann operators [10]. The Pauli's form an orthogonal basis in $L(\mathbb{C}^2)$ under the Hilbert-Schmidt inner product. They are unitary, Hermitian and traceless. The generalized Gell-Mann operators satisfy all of these properties except unitarity, which will not be of concern to us. We will assume that each operator in the basis, $\{P_a\}$, $a \in \{0, \dots, D^2 - 1\}$, is appropriately scaled so that,

$$[P_a P_b] = D\delta_{a,b}. \quad (8)$$

Note that Hermiticity of the basis implies $\forall a$,

$$P_a^T = P_a^*. \quad (9)$$

We will use the convention $P_0 = \mathbb{1}$.

2.3 Permutation Operators and the Symmetric Subspace

We briefly discuss permutation operators and the symmetric subspace, and then present some results regarding them that will be used later. Let $\mathcal{H}^{\otimes k}$ be a k -fold tensor product of the Hilbert space \mathcal{H} . If S_k is the symmetric group on k objects and $\sigma \in S_k$ then the unitary permutation operator P_σ is defined by

$$P_\sigma (|u_1\rangle \otimes \dots \otimes |u_k\rangle) = |u_{\sigma^{-1}(1)}\rangle \otimes \dots \otimes |u_{\sigma^{-1}(k)}\rangle \quad (10)$$

where the $|u_i\rangle$ are arbitrary elements of \mathcal{H} . The symmetric subspace for $\mathcal{H}^{\otimes k}$ is the set of all states that are invariant under any such permutation operator. Denoting the projector onto the symmetric subspace by $\pi_{\text{sym}}(k, D)$ we have,

$$\pi_{\text{sym}}(k, D) = \frac{1}{k!} \sum_{\sigma \in S_k} P_\sigma. \quad (11)$$

Next we discuss a useful result regarding traces of permutation operators multiplied by arbitrary tensor products. Suppose that we have k operators A_1, \dots, A_k each of which are in $L(\mathcal{H})$. As well, suppose that P_σ is the unitary permutation operator corresponding to the permutation $\sigma \in S_k$. Up to ordering, every permutation in S_k can be written in cyclic form, that is, it can be written as a product of simple cycles. Let σ be written in its cyclic form as $(a_1 \dots a_r) \dots (a_q \dots a_k)$ so that there is a one to one mapping between the a_j and the set $\{1, \dots, k\}$. Then,

$$[(A_1 \otimes \dots \otimes A_k) P_\sigma] = [A_{a_1} \dots A_{a_r}] \dots [A_{a_q} \dots A_{a_k}]. \quad (12)$$

Pictorially this means that to calculate $[(A_1 \otimes \dots \otimes A_k) P_\sigma]$ one just writes σ in its cyclic decomposition, places each A_i element in the unique spot that i occurs in the cyclic decomposition and replaces each set of “()” with “[]”.

The following result [16] will also be important in the calculation of the second moment of the fidelity,

$$\int (|\psi\rangle\langle\psi|)^{\otimes k} d\psi = \frac{\pi_{\text{sym}}(k, d)}{[\pi_{\text{sym}}(k, d)]}. \quad (13)$$

2.4 The Choi-Jamiolkowski State for a Quantum Operation

For a quantum operation Λ acting on $L(\mathcal{H})$, the Choi-Jamiolkowski state for Λ [4] is the positive trace-1 operator $J(\Lambda)$ in $L(\mathcal{H} \otimes \mathcal{H})$ given by,

$$J(\Lambda) = \sum_{(a,b) \in \mathbb{Z}_D \times \mathbb{Z}_D} \Lambda(|a\rangle\langle b|) \otimes |a\rangle\langle b|. \quad (14)$$

If we denote the maximally entangled Bell state on $\mathcal{H} \otimes \mathcal{H}$ by σ then,

$$J(\Lambda) = \Lambda \otimes \mathcal{I}(D\sigma). \quad (15)$$

Since Λ is a quantum operation, $\frac{J(\Lambda)}{D}$ is a quantum state [4]. This correspondence is a bijection between quantum operations and states. For the rest of the paper we will denote $\frac{J(\Lambda)}{D}$ by J .

3 Calculating the Variance of the Gate Fidelity

Let \mathcal{E} and unitary \mathcal{U} be arbitrary quantum and unitary operations respectively. In this section we will explicitly calculate the variance of $\mathcal{F}_{\mathcal{E},\mathcal{U}} : (\mathbb{C}\mathbb{P}^{D-1}, \|\cdot\|_2) \rightarrow \mathbb{R}$,

$$\text{Var}(\mathcal{F}_{\mathcal{E},\mathcal{U}}) = \overline{\mathcal{F}_{\mathcal{E},\mathcal{U}}^2} - \overline{\mathcal{F}_{\mathcal{E},\mathcal{U}}^2}, \quad (16)$$

in terms of both the Kraus operators and χ -matrix (see below) for $\Lambda = \mathcal{U}^\dagger \circ \mathcal{E}$. The χ -matrix for Λ is a D^2 by D^2 matrix of complex numbers that completely describes Λ once a basis for $L(\mathbb{C}^D)$ is fixed [5]. It is a useful object in quantum state estimation [1] because any element of χ can be estimated efficiently, with estimation of the off-diagonal elements requiring only a single clean ancillary qubit.

The method by which we calculate $\overline{\mathcal{F}_{\mathcal{E},\mathcal{U}}^2}$ is a specific case of a method that calculates all moments of $\mathcal{F}_{\mathcal{E},\mathcal{U}}$. Therefore, in order to gain some intuition for the method, and compare it with known results, we first calculate $\overline{\mathcal{F}_{\mathcal{E},\mathcal{U}}}$. To make equations less cumbersome we will denote $\mathcal{F}_{\mathcal{E},\mathcal{U}}$ by \mathcal{F} .

3.1 Average Fidelity

By definition,

$$\begin{aligned} \mathcal{F}(|\psi\rangle\langle\psi|) &= [\Lambda(|\psi\rangle\langle\psi|)|\psi\rangle\langle\psi|] = \sum_i \langle\psi|K_i|\psi\rangle\langle\psi|K_i^\dagger|\psi\rangle \\ &= \sum_i [K_i|\psi\rangle\langle\psi|] [K_i^\dagger|\psi\rangle\langle\psi|] \\ &= \sum_i \left[(K_i \otimes K_i^\dagger) |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \right]. \end{aligned} \quad (17)$$

Therefore,

$$\begin{aligned} \overline{\mathcal{F}} &= \int \mathcal{F}(|\psi\rangle\langle\psi|) d\psi = \sum_i \left[(K_i \otimes K_i^\dagger) \int |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| d\psi \right] \\ &= \sum_i \left[(K_i \otimes K_i^\dagger) \frac{\pi_{\text{sym}}(2, D)}{[\pi_{\text{sym}}(2, D)]} \right], \end{aligned} \quad (18)$$

since $\int |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| d\psi = \frac{\pi_{\text{sym}}(2, D)}{[\pi_{\text{sym}}(2, D)]}$. Hence using $\pi_{\text{sym}}(2, D) = \frac{1}{2} \sum_{\sigma \in S_2} P_\sigma$ and the result on taking traces of tensor products of operators with permutation operators,

$$\begin{aligned} \overline{\mathcal{F}} &= \frac{1}{2[\pi_{\text{sym}}(2, D)]} \sum_i \sum_{\sigma \in S_2} \left[(K_i \otimes K_i^\dagger) P_\sigma \right] \\ &= \frac{1}{2[\pi_{\text{sym}}(2, D)]} \left(\sum_i ([K_i][K_i^\dagger]) + D \right). \end{aligned} \quad (19)$$

Since

$$\begin{aligned}
[\pi_{\text{sym}}(2, D)] &= [(\mathbb{1} \otimes \mathbb{1}) \pi_{\text{sym}}(2, D)] \\
&= \frac{D^2 + D}{2}
\end{aligned} \tag{20}$$

we have the well-known result,

$$\bar{\mathcal{F}} = \frac{\sum_i ([K_i][K_i^\dagger]) + D}{D^2 + D}. \tag{21}$$

This can be further simplified if we expand the K_i in terms of the generalized Gell-Mann basis $\{P_i\}$. Suppose $K_i = \sum_j \gamma_j^i P_j$ so that,

$$\begin{aligned}
\Lambda(\rho) &= \sum_i \left(\sum_l \gamma_l^i P_l \right) \rho \left(\sum_m (\gamma_m^i)^* P_m \right) \\
&= \sum_{l,m} \left(\sum_i \gamma_l^i (\gamma_m^i)^* \right) P_l \rho P_m.
\end{aligned} \tag{22}$$

The coefficients $\sum_i \gamma_l^i (\gamma_m^i)^*$ form a D^2 by D^2 matrix that is commonly called the χ matrix. Thus we have,

$$\Lambda(\rho) = \sum_{l,m} \chi_{l,m} P_l \rho P_m. \tag{23}$$

Hence we can write the average fidelity as,

$$\begin{aligned}
\bar{\mathcal{F}} &= \frac{1}{D^2 + D} \sum_i \left[\left(\sum_l \gamma_l^i P_l \otimes \sum_m \gamma_m^i P_m \right) \pi_{\text{sym}}(2, D) \right] \\
&= \frac{1}{D^2 + D} \sum_{l,m} \left(\sum_i \gamma_l^i \gamma_m^i \right) [(P_l \otimes P_m) \pi_{\text{sym}}(2, D)] \\
&= \frac{1}{D^2 + D} \sum_{l,m} \chi_{l,m} ([P_l][P_m] + [P_l P_m]) \\
&= \frac{\chi_{0,0} D + 1}{D + 1}.
\end{aligned} \tag{24}$$

Next we calculate the variance of the gate fidelity using analogous methods.

3.2 Variance of the Fidelity

By definition,

$$\begin{aligned}
\mathcal{F}^2(|\psi\rangle\langle\psi|) &= [\Lambda(|\psi\rangle\langle\psi|)|\psi\rangle\langle\psi|] [\Lambda(|\psi\rangle\langle\psi|)|\psi\rangle\langle\psi|] \\
&= \sum_i \langle\psi|K_i|\psi\rangle\langle\psi|K_i^\dagger|\psi\rangle \sum_i \langle\psi|K_j|\psi\rangle\langle\psi|K_j^\dagger|\psi\rangle \\
&= \sum_i \left[(K_i \otimes K_i^\dagger) |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \right] \sum_j \left[(K_j \otimes K_j^\dagger) |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \right] \\
&= \sum_{i,j} \left[(K_i \otimes K_i^\dagger \otimes K_j \otimes K_j^\dagger) |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \right]. \tag{25}
\end{aligned}$$

Therefore,

$$\begin{aligned}
\overline{\mathcal{F}^2} &= \sum_{i,j} \text{tr} \left[(K_i \otimes K_i \otimes K_j \otimes K_j) \overline{|\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi|} \right] \\
&= \sum_{i,j} \left[(K_i \otimes K_i^\dagger \otimes K_j \otimes K_j^\dagger) \frac{\pi_{\text{sym}}(4, D)}{[\pi_{\text{sym}}(4, D)]} \right] \tag{26}
\end{aligned}$$

since $\overline{|\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi|} = \frac{\pi_{\text{sym}}(4, D)}{[\pi_{\text{sym}}(4, D)]}$. Using $\pi_{\text{sym}}(4, D) = \frac{1}{24} \sum_{\sigma \in S_4} P_\sigma$ and the result regarding taking traces of tensor products of operators with permutation operators we have,

$$\begin{aligned}
\overline{\mathcal{F}^2} &= \frac{1}{24 [\pi_{\text{sym}}(4, D)]} \sum_{i,j} \sum_{\sigma \in S_4} \left[(K_i \otimes K_i^\dagger \otimes K_j \otimes K_j^\dagger) P_\sigma \right] \\
&= \sum_{i,j} \frac{[K_i][K_i^\dagger][K_j][K_j^\dagger] + [K_i K_j^\dagger][K_i^\dagger][K_j] + \dots}{24 [\pi_{\text{sym}}(4, D)]} \tag{27}
\end{aligned}$$

where there are 24 terms in the sum corresponding to the $4!$ permutations of 4 objects. Again, we can write $\overline{\mathcal{F}^2}$ by expanding the K_i in terms of the generalized Gell-Mann basis. Suppose $K_i = \sum_j \gamma_j^i P_j$. Then,

$$\begin{aligned}
\left[(K_i \otimes K_i^\dagger \otimes K_j \otimes K_j^\dagger) \pi_{\text{sym}}(4, D) \right] &= \left[\left(\sum_l \gamma_l^i P_l \otimes \sum_m \gamma_m^i{}^* P_m \otimes \sum_n \gamma_n^j P_n \otimes \sum_r \gamma_r^j{}^* P_r \right) \pi_{\text{sym}}(4, D) \right] \\
&= \sum_{l,m,n,r} \gamma_l^i \gamma_m^i{}^* \gamma_n^j \gamma_r^j{}^* [(P_l \otimes P_m \otimes P_n \otimes P_r) \pi_{\text{sym}}(4, D)]. \tag{28}
\end{aligned}$$

Hence,

$$\begin{aligned}
\overline{\mathcal{F}^2} &= \frac{1}{[\pi_{\text{sym}}(4, D)]} \sum_{l,m,n,r} \left(\sum_{i,j} \gamma_l^i \gamma_m^i{}^* \gamma_n^j \gamma_r^j{}^* \right) [(P_l \otimes P_m \otimes P_n \otimes P_r) \pi_{\text{sym}}(4, D)] \\
&= \frac{1}{[\pi_{\text{sym}}(4, D)]} \sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} [(P_l \otimes P_m \otimes P_n \otimes P_r) \pi_{\text{sym}}(4, D)] \\
&= \frac{1}{24 [\pi_{\text{sym}}(4, D)]} \sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l][P_m][P_n][P_r] + [P_l P_r][P_m][P_n] + \dots) \tag{29}
\end{aligned}$$

Since,

$$\begin{aligned}
[\pi_{\text{sym}}(4, D)] &= \frac{[\mathbb{1}][\mathbb{1}][\mathbb{1}][\mathbb{1}] + [\mathbb{1}\mathbb{1}][\mathbb{1}][\mathbb{1}] + \dots}{24} \\
&= \frac{D^4 + 6D^3 + 11D^2 + 6D}{24}, \tag{30}
\end{aligned}$$

a direct calculation using the previously discussed properties of the generalized Gell-Mann basis gives,

$$\begin{aligned}
\overline{\mathcal{F}^2} &= \frac{1}{D^4 + 6D^3 + 11D^2 + 6D} \left(\chi_{0,0}^2 D^4 + D^3 \left(2(\chi^2)_{0,0} + (\chi\chi^T)_{0,0} + (\chi^T\chi)_{0,0} + 2\chi_{0,0} \right) \right. \\
&\quad + D^2 \left(4\chi_{0,0} + [\chi\chi^T] + 2 \left[\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \Lambda \left(\frac{\mathbb{1}}{D} \right) \right] + [\chi^2] \right. \\
&\quad \left. \left. + 1 + \left[\left(\Lambda(\mathbb{1}) \right)^2 \right] \right) + 3D + 2 \left[\sum_{l,m} \chi_{l,m} P_l \Lambda(P_m) \right] \right). \tag{31}
\end{aligned}$$

Using $\overline{\mathcal{F}^2} = \frac{\chi_{0,0}^2 D^2 + 2\chi_{0,0} D + 1}{D^2 + 2D + 1}$ we have an expression for $\overline{\mathcal{F}^2} - \mathcal{F}^2$ in terms of the χ -matrix for Λ ,

$$\begin{aligned}
\text{Var}(\mathcal{F}) &= \frac{1}{D(D^2 + 2D + 1)(D^2 + 5D + 1)} \left(D^4 \left(-4\chi_{0,0}^2 + (\chi^T\chi)_{0,0} + (\chi\chi^T)_{0,0} + 2(\chi^2)_{0,0} \right) \right. \\
&\quad + D^3 \left(-6\chi_{0,0}^2 + (\chi^T\chi)_{0,0} + (\chi\chi^T)_{0,0} + [\chi\chi^T] + 2 \left[\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \Lambda \left(\frac{\mathbb{1}}{D} \right) \right] \right. \\
&\quad \left. \left. - 4\chi_{0,0} + [\chi^2] + 2(\chi^2)_{0,0} + \left[\left(\Lambda \left(\frac{\mathbb{1}}{D} \right) \right)^2 \right] \right) \right. \\
&\quad + D^2 \left(-8\chi_{0,0} + [\chi^2] + [\chi\chi^T] - 1 + 2 \left[\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \Lambda \left(\frac{\mathbb{1}}{D} \right) \right] + \left[\left(\Lambda \left(\frac{\mathbb{1}}{D} \right) \right)^2 \right] \right) \\
&\quad \left. + D \left(2 \left[\sum_{l,m} \chi_{l,m} P_l \Lambda(P_m) \right] - 3 \right) + 2 \left[\sum_{l,m} \chi_{l,m} P_l \Lambda(P_m) \right] \right). \tag{32}
\end{aligned}$$

Next we discuss the extension of the methods used in this section to higher order moments.

4 Higher Order Moments

For $m \in \mathbb{N}$, \mathcal{F}^m has action given by,

$$\begin{aligned}
\mathcal{F}^m (|\psi\rangle\langle\psi|) &= [\Lambda (|\psi\rangle\langle\psi|) |\psi\rangle\langle\psi|]^m \\
&= \sum_{i_1} \left[\left(K_{i_1} \otimes K_{i_1}^\dagger \right) |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \right] \dots \sum_{i_m} \left[\left(K_{i_m} \otimes K_{i_m}^\dagger \right) |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \right] \\
&= \sum_{i_1, \dots, i_m} \left[\left(K_{i_1} \otimes K_{i_1}^\dagger \otimes \dots \otimes K_{i_m} \otimes K_{i_m}^\dagger \right) |\psi\rangle\langle\psi|^{\otimes m} \right]. \tag{33}
\end{aligned}$$

Hence using the previous results on permutation operators and the symmetric subspace,

$$\begin{aligned}
\overline{\mathcal{F}^m} &= \frac{1}{[\pi_{sym}(2m, D)]} \sum_{i_1, \dots, i_m} \left[\left(K_{i_1} \otimes K_{i_1}^\dagger \otimes \dots \otimes K_{i_m} \otimes K_{i_m}^\dagger \right) \pi_{sym}(2m, D) \right] \\
&= \frac{1}{(2m)! \binom{2m+D-1}{D-1}} \sum_{i_1, \dots, i_m} [K_{i_1}] [K_{i_1}^\dagger] \dots [K_{i_m}] [K_{i_m}^\dagger] + \dots + [K_{i_1} K_{i_1}^\dagger \dots K_{i_m} K_{i_m}^\dagger] \tag{34}
\end{aligned}$$

with $(2m)!$ terms in the sum corresponding to the fact that there are $(2m)!$ elements in the symmetric group S_{2m} . We have also used the fact that,

$$[\pi_{sym}(2m, D)] = \binom{2m+D-1}{D-1}. \tag{35}$$

Expanding in terms of the generalized Gell-Mann basis gives,

$$\begin{aligned}
\overline{\mathcal{F}^m} &= \frac{1}{(2m)! \binom{2m+D-1}{D-1}} \sum_{i_1, i_2, \dots, i_{m_1}, i_{m_2}} \chi_{i_1, i_2} \dots \chi_{i_{m_1}, i_{m_2}} ([P_{i_1}] [P_{i_2}] \dots [P_{i_{m_1}}] [P_{i_{m_2}}] + \dots) \\
&= \frac{1}{(2m)! \binom{2m+D-1}{D-1}} (\chi_{0,0}^m D^{2m} + \dots), \tag{36}
\end{aligned}$$

Next we use the expressions obtained for $\overline{\mathcal{F}^2}$ and $\overline{\mathcal{F}}$ in terms of the χ -matrix to obtain expressions for these quantities in terms of the Choi-Jamiolkowski state for Λ .

5 Variance in Terms of the Choi-Jamiolkowski State

The two expressions we have given for $\overline{\mathcal{F}^2}$ to this point are in terms of the Kraus operators (27) and χ -matrix (31) for Λ . In this section we use (31) to obtain an expression in terms of the Choi-Jamiolkowski state for Λ . One advantage of this representation is that it is basis independent unlike the χ -matrix representation that was obtained by expanding the Kraus operators in terms of the generalized Gell-Mann basis. Another advantage is that this expression allows for a simple method to calculate the time evolution of the variance for Markovian noise, as will be discussed below.

Let J be the Choi-Jamiolkowski state for Λ and σ be the maximally entangled Bell state $|\psi_0\rangle\langle\psi_0|$ on $\mathcal{H} \otimes \mathcal{H}$ where,

$$|\psi_0\rangle = \frac{1}{\sqrt{D}} \sum_{i=0}^{D-1} |i\rangle \otimes |i\rangle. \tag{37}$$

The details of the calculation of both $\overline{\mathcal{F}^2}$ and $\overline{\mathcal{F}^2}$ are given in the appendix. For $\overline{\mathcal{F}}$ we get,

$$\overline{\mathcal{F}} = \frac{[J\sigma]D + 1}{D + 1} \quad (38)$$

which implies

$$\overline{\mathcal{F}^2} = \frac{[J\sigma]^2 D^2 + 2[J\sigma]D + 1}{D^2 + 2D + 1}. \quad (39)$$

The expression for $\overline{\mathcal{F}^2}$ is,

$$\begin{aligned} \overline{\mathcal{F}^2} = & \frac{1}{D^4 + 6D^3 + 11D^2 + 6D} \left([J\sigma]^2 D^4 + D^3 (2[J^2\sigma] + [JJ^T\sigma] + [J^T J\sigma] + 2[J\sigma]) \right. \\ & + D^2 \left(4[J\sigma] + [JJ^T] + 2D [J\sigma + \sigma J]^{T_2} [J]^{T_2} \right) + [J^2] \\ & \left. + 1 + \left(([J]^{T_2})^2 \right) \right) + 3D + 2D^4 \left[(J\sigma^{T_2})^\dagger (J\sigma^{T_2})^{T_2} \right]. \end{aligned} \quad (40)$$

where $(\cdot)^{T_2}$ denotes the partial transpose with respect to the second subsystem and $[\cdot]^{T_2}$ refers to the partial trace over the second subsystem. Thus, (39) and (40) together give an expression for the $\text{Var}\mathcal{F}$ in terms of J .

5.1 Time Dependent Markovian Noise

As mentioned previously, an expression for $\text{Var}\mathcal{F}$ in terms of J reduces the time-complexity of determining the time evolution of the variance of the gate fidelity between Markovian noise $\Lambda(t)$ and the identity operation \mathcal{I} . Suppose $\Lambda(t)$ is Markovian and $t \geq 0$. Markovicity implies that $\Lambda(t)$ satisfies the semigroup property,

$$\Lambda(t_1 + t_2) = \Lambda(t_1) \circ \Lambda(t_2) \quad (41)$$

$\forall t_1, t_2 \geq 0$. This implies that if one has a description for $\Lambda(\Delta t)$ for some Δt then for any $m \geq 1$ they have a description of the noise at $m\Delta t$ by taking the m -fold composition of $\Lambda(\Delta t)$ with itself. We denote this m -fold composition by $(\Lambda(\Delta t))^m$. By the definition of the Choi-Jamiolkowski state,

$$\begin{aligned} J(m\Delta t) &= \sum_{(a,b) \in \mathbb{Z}_D \times \mathbb{Z}_D} \Lambda(m\Delta t) (|a\rangle\langle b| \otimes |a\rangle\langle b|) \\ &= \sum_{(a,b) \in \mathbb{Z}_D \times \mathbb{Z}_D} (\Lambda(\Delta t))^m (|a\rangle\langle b| \otimes |a\rangle\langle b|) \\ &= \Lambda(\Delta t) \otimes \mathcal{I} \left(\sum_{(a,b) \in \mathbb{Z}_D \times \mathbb{Z}_D} (\Lambda(\Delta t))^{m-1} (|a\rangle\langle b| \otimes |a\rangle\langle b|) \right) \\ &= \Lambda(\Delta t) \otimes \mathcal{I}(J((m-1)\Delta t)). \end{aligned} \quad (42)$$

Therefore if one has the expression for $\Lambda(\Delta t)$ they have $J(m\Delta t)$ for any $m \geq 1$ by just acting $\Lambda(\Delta t)$ on the first subsystem m times. In moving from $(m-1)\Delta t$ to $m\Delta t$ one need only update the Choi-Jamiolkowski state using $J(\Delta t)$ and calculate a fixed number of traces. Hence, using the representation of the variance in terms of the Choi-Jamiolkowski state, the complexity of calculating the variance does not increase in time for Markovian noise. If one uses only $\Lambda(\Delta t)$ to calculate the variance using the Kraus representation then one would have to either find a Kraus representation at each time step or have the number of traces increases as the square of the number of Kraus operators for Λ at each time step. Since composition of quantum operations does not correspond to composition of the associated χ -matrices, the χ -matrix would also have to be re-evaluated at each time step. Next we look at the case of a single qubit.

6 Variance For a Single Qubit

In the case of a single qubit we can obtain a more simple expression for the variance. The calculation is contained in the appendix and for $\overline{\mathcal{F}^2}$ we get,

$$\overline{\mathcal{F}^2} = \frac{\left(-48\chi_{0,0}^2 + 64\chi_{0,0} + 16(\chi\chi^T + \chi^T\chi)_{0,0} + 16(\chi^2)_{0,0} + 4[\chi\chi^T] + 12[\chi^2] + 8 + [\Lambda(\mathbb{1})^2] \right)}{120}. \quad (43)$$

Since $\overline{\mathcal{F}^2} = \frac{\chi_{0,0}^2 D^2 + 2\chi_{0,0} D + 1}{D^2 + 2D + 1}$ we have,

$$\overline{\mathcal{F}^2} = \frac{\left(4\chi_{0,0}^2 + 4\chi_{0,0} + 1 \right)}{9}. \quad (44)$$

Thus in terms of the χ -matrix and Choi-Jamiolkowski state for Λ we get the particularly simple expressions,

$$\begin{aligned} \overline{\mathcal{F}^2} - \overline{\mathcal{F}}^2 &= \frac{-38}{45}\chi_{0,0}^2 + \frac{4}{45}\chi_{0,0} - \frac{2}{45} + \frac{1}{120} \left(16 \left((\chi\chi^T)_{0,0} + (\chi^T\chi)_{0,0} \right) \right. \\ &\quad \left. + 16(\chi^2)_{0,0} + 4[\chi\chi^T] + 12[\chi^2] + [\Lambda(\mathbb{1})^2] \right) \\ &= \frac{-38}{45}[J\sigma]^2 + \frac{4}{45}[J\sigma] - \frac{2}{45} + \frac{1}{120} \left(16 \left([JJ^T\sigma] + [J^T J\sigma] \right) \right. \\ &\quad \left. + 16[J^2\sigma] + 4[JJ^T] + 12[J^2] + \left[([J]^{T_2})^2 \right] \right). \end{aligned} \quad (45)$$

Next we look at the behavior of \mathcal{F} for large dimensional quantum systems.

7 Behaviour for Large Dimensional Quantum Systems

The denominator of (32) is a quintic polynomial in the dimension D . The numerator contains powers of D up to and including 4, however the coefficients depend on the χ -matrix. We would like to bound these coefficients in terms of D .

First, since χ is a trace-1 positive semi-definite matrix, $\chi_{0,0} \leq 1$ and $[\chi^2] \leq [\chi] = 1$. The Frobenius (Hilbert-Schmidt) norm on $L(\mathbb{C}^D)$, denoted by $\|\cdot\|_F$, is the operator norm induced by the Hilbert-Schmidt inner product. Explicitly, for $A \in L(\mathbb{C}^D)$, $\|A\|_F = \sqrt{\text{tr}(A^\dagger A)}$. Using the by the Cauchy-Schwarz inequality,

$$|[\chi\chi^T]| \leq \|\chi\|_F \|\chi^T\|_F. \quad (46)$$

Since χ and χ^T have the same singular values $\|\chi\|_F = \|\chi^T\|_F$. Therefore since $\|\chi\|_F \leq 1$ we get $|[\chi\chi^T]| \leq 1$. This also implies $(\chi\chi^T)_{0,0} \leq 1$ and $(\chi^T\chi)_{0,0} \leq 1$. Next, note that since $\Lambda\left(\frac{1}{D}\right)$ is trace-1 and positive semi-definite, $\left[\Lambda\left(\frac{1}{D}\right)\right]^2 \leq 1$.

The only two coefficients that remain to be bounded are $\left[\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \Lambda\left(\frac{1}{D}\right)\right]$ and $\left[\sum_{l,m} \chi_{l,m} P_l \Lambda(P_m)\right]$. By the Cauchy-Schwarz inequality,

$$\begin{aligned} \left| \left[\sum_l \chi_{l,0} P_l \Lambda\left(\frac{1}{D}\right) \right] \right| &\leq \left\| \sum_l \chi_{l,0} P_l \right\|_F \left\| \Lambda\left(\frac{1}{D}\right) \right\|_F \\ &\leq \left\| \sum_l \chi_{l,0} P_l \right\|_F. \end{aligned} \quad (47)$$

Since,

$$\begin{aligned} \left\| \sum_l \chi_{l,0} P_l \right\|_F &= \sqrt{\left[\left(\sum_l \chi_{l,0} P_l \right)^\dagger \left(\sum_m \chi_{m,0} P_m \right) \right]} = \sqrt{\left[\left(\sum_l \chi_{0,l} P_l \right) \left(\sum_m \chi_{m,0} P_m \right) \right]} \\ &= D (\chi^2)_{0,0} \\ &\leq D. \end{aligned} \quad (48)$$

we get $\left[\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \Lambda\left(\frac{1}{D}\right)\right] \leq 2D$.

Finally, using $\left[\sum_{l,m} \chi_{l,m} P_l \Lambda(P_m)\right] = D^2 \left[S(SJ)^{T_1} J \right]$ from the appendix we would like to bound $\left[JS(SJ)^{T_1} \right]$. Again using the Cauchy-Schwarz inequality,

$$\begin{aligned} \left| \left[JS(SJ)^{T_1} \right] \right| &\leq \|JS\|_F \|(SJ)^{T_1}\|_F \\ &= \sqrt{[(JS)(JS)^\dagger]} \sqrt{\left[\left((SJ)^{T_1} \right)^\dagger (SJ)^{T_1} \right]} \\ &\leq \sqrt{\left[\left((SJ)^{T_1} \right)^\dagger (SJ)^{T_1} \right]} \end{aligned} \quad (49)$$

since $\sqrt{[(JS)(JS)^\dagger]} = \sqrt{[J^2]} = \|J\|_F \leq 1$. Now for any $A, B \in L(\mathcal{H} \otimes \mathcal{H})$ we have that $(A^\dagger)^{T_1} = (A^{T_1})^\dagger$ and $[(AB)^{T_1}] = [B^{T_1}A^{T_1}]$. Thus,

$$\begin{aligned} \left[\left((SJ)^{T_1} \right)^\dagger (SJ)^{T_1} \right] &= \left[\left((SJ)^\dagger \right)^{T_1} (SJ)^{T_1} \right] = \left[(SJ)^{T_1} \left((SJ)^\dagger \right)^{T_1} \right] \\ &= \left[\left((SJ)^\dagger (SJ) \right)^{T_1} \right] \\ &= [J^2] \\ &\leq 1, \end{aligned} \tag{50}$$

which implies $\left[\sum_{l,m} \chi_{l,m} P_l \Lambda(P_m) \right] \leq D^2$. Thus, the numerator of (32) is quartic in D .

This implies that for large D we can write,

$$\begin{aligned} \overline{\mathcal{F}^2} - \overline{\mathcal{F}}^2 &\sim \frac{O(D^3)}{O(D^4)} \\ &\sim O\left(\frac{1}{D}\right) \end{aligned} \tag{51}$$

and so $\overline{\mathcal{F}^2} - \overline{\mathcal{F}}^2 \rightarrow 0$ as $\frac{1}{D}$ when $D \rightarrow \infty$.

8 Discussion

We have given a method for calculating all moments of the gate fidelity $\mathcal{F}_{\mathcal{E},\mathcal{U}}$ between a unitary \mathcal{U} and a quantum operation \mathcal{E} . A consequence of this is that we obtain various closed form expressions for $\text{Var}(\mathcal{F}_{\mathcal{E},\mathcal{U}})$. Using these expressions we have obtained a simple expression in the case of a single qubit and have shown that for large quantum systems, the variance is $O\left(\frac{1}{D}\right)$. The expression for $\text{Var}(\mathcal{F}_{\mathcal{E},\mathcal{U}})$ in terms of the Choi-Jamiolkowski state can be used to look at the time evolution of the variance of $\mathcal{F}_{\mathcal{E},\mathcal{I}}$ in the case of Markovian noise.

There is growing interest in the use of twirling [3, 6] and randomization methods [7, 12] to estimate partial information about the unknown noise affecting the implementation of quantum memory or quantum gates in a completely scalable manner [8, 17]. In addition to the eigenvalues of the twirled noisy operation (which includes the average gate fidelity as a special case), it is hoped that other information such as the variance of the fidelity over the twirling/randomizing gate set may provide useful information about the unknown noise model. Indeed in [12] it is suggested that the variance of the fidelity measured under the proposed randomized benchmarking protocol may provide useful information about the extent to which the noise is coherent. Our work shows that there are a number of difficulties with analyzing the variance of the fidelity in this context.

First, we observe that the variance decreases exponentially with the number of qubits that are involved in the randomized benchmarking or twirling protocol. This implies that an exponentially increasing number of repetitions of the protocol would be required to obtain a reliable estimate of the variance. Secondly, we remark that in order for the variance to be independent of the initial state and the particular choice of randomizing gates (and hence reflect some intrinsic feature of

the noise model), the randomizing gates must comprise (or at least generate) a unitary 4-design. Since the Clifford group is only a unitary 2-design (see in particular [6] for further discussion), randomizing under different choices of Clifford gate sets can produce different values for the variance. However, the original randomized benchmarking protocol considered in [7], which suggested using Haar-random gates, will produce a variance that depends only on the noise model (assuming, as usual, that the noise is effectively independent of the sequence of randomizing gates). While that protocol may be practical for single qubits, or a small numbers of qubits, the fact that exponential complexity is required to implement a Haar-random unitary makes the protocol of [7] impractical for large numbers of qubits.

Lastly, even under a benchmarking protocol for a single qubit that makes use of a gate set that generates a 4-design, our expression shows that the variance depends in a non-trivial way on both the diagonal and off-diagonal elements of the χ -matrix. Hence the extent of the coherence of the noise model, understood here as referring to the fact that the noise can not be expressed as a Pauli channel, can not be inferred from an estimate of the variance alone. However, there remains the possibility that the extent of coherence in the noise could be estimated by comparing results from different randomized benchmarking schemes, eg. with and without supplementary Pauli rotations. This would be a worthwhile topic for further investigation.

As a final comment, another application of our results is in the context of simulating quantum systems on a quantum computer. This one of the most important potential applications of quantum information processing, and the most likely to be possible in the near term. Of course an important shortcoming of efficient quantum simulation (relative to inefficient simulation on a classical computer) is that not all the information about the simulated system is available upon measurement. This “readout problem” poses a practical obstacle and opens the question of what, if any, properties of the system may be estimated with a scalable number of repetitions of the simulation.

In the context of studying quantum chaos, it was suggested in [9] that the characteristics of fidelity decay under perturbation, an important indicator of quantum chaos, could be estimated in an efficient manner. In particular, under the random matrix conjecture for complex and chaotic systems, the fidelity decay can be predicted exactly under any known perturbation, and compared to the observed decay. An implicit assumption of that argument is that the variance of the fidelity remains small as the system dimension increases so that a reliable estimate of the mean is possible with a scalable number of repetitions. Our result on bounding the variance shows that this is indeed the case and gives a rigorous justification to that work.

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10 Appendix

10.1 Gate Fidelity in terms of the Choi-Jamiolkowski Operator

10.1.1 Relating the χ -matrix to the Choi-Jamiolkowski operator

The first step in obtaining an expression for the variance in terms of the Choi-Jamiolkowski state J for Λ is to find a relationship between the χ -matrix and J . If we define the orthonormal basis

$\{|\psi_0\rangle, \dots, |\psi_{D^2-1}\rangle\}$ by,

$$|\psi_i\rangle = P_i \otimes \mathbb{1}|\psi_0\rangle. \quad (52)$$

$\forall i \in \{0, \dots, D^2 - 1\}$ where $\{P_i\}$ is the generalized Gell-Mann basis then with respect to the basis $\mathcal{B} = \{|\psi_i\rangle\langle\psi_j| : i, j \in \{0, \dots, D^2 - 1\}\}$ for $L(\mathcal{H} \otimes \mathcal{H})$,

$$J_{l,m} = \chi_{l,m}. \quad (53)$$

To see this first note that,

$$\sigma = |\psi_0\rangle\langle\psi_0| = \frac{1}{D^2} \sum_{k=0}^{D^2-1} P_k^T \otimes P_k = \frac{1}{D^2} \sum_{k=0}^{D^2-1} P_k \otimes P_k^T. \quad (54)$$

Since $\Lambda(\rho) = \sum_{l,m} \chi_{l,m} P_l \rho P_m$ and $J = \Lambda \otimes \mathcal{I}(\sigma)$ we get,

$$J = \frac{1}{D^2} \sum_{k,l,m} \chi_{l,m} (P_l P_k P_m \otimes P_k^T). \quad (55)$$

Then we have,

$$\begin{aligned} J_{n,q} = \langle\psi_n|J|\psi_q\rangle &= [(P_n \otimes \mathbb{1})J(P_q \otimes \mathbb{1})|\psi_0\rangle\langle\psi_0|] \\ &= \frac{1}{D^4} \sum_{j,k,l,m} \chi_{l,m} [P_q P_j P_n P_l P_k P_m] [P_j^T P_k^T] \\ &= \frac{1}{D^3} \sum_{k,l,m} \chi_{l,m} [P_q P_k P_n P_l P_k P_m]. \end{aligned} \quad (56)$$

Since $[P_i P_j] = D\delta_{i,j}$, for any $A \in L(\mathbb{C}^D)$,

$$\sum_{k=0}^{D^2-1} P_k A P_k = D[A] \mathbb{1}. \quad (57)$$

Hence,

$$J_{n,q} = \frac{1}{D^3} \sum_{l,m} \chi_{l,m} [P_q (D[P_n P_l] \mathbb{1}) P_m] = \chi_{n,q} \quad (58)$$

and $\chi_{0,0} = [J\sigma]$.

We can now express $\overline{\mathcal{F}}^2$ as

$$\overline{\mathcal{F}}^2 = \frac{[J\sigma]^2 D^2 + 2[J\sigma]D + 1}{D^2 + 2D + 1} \quad (59)$$

and for $\overline{\mathcal{F}}^2$ with $\Lambda\left(\frac{\mathbb{1}}{D}\right) = [J]^{T_2}$ we get,

$$\begin{aligned}
\overline{\mathcal{F}^2} &= \frac{1}{D^4 + 6D^3 + 11D^2 + 6D} \left([J\sigma]^2 D^4 + D^3 (2 [J^2\sigma] + [JJ^T\sigma] + [J^T J\sigma] + 2 [J\sigma]) \right. \\
&\quad + D^2 \left(4 [J\sigma] + [JJ^T] + 2 \left(\sum_l (\chi_{l,0} + \chi_{0,l}) \left[P_l \Lambda \left(\frac{\mathbb{1}}{D} \right) \right] \right) + [J^2] \right. \\
&\quad \left. \left. + 1 + \left[([J]^{T_2})^2 \right] \right) + 3D + 2 \sum_{l,m} \chi_{l,m} [P_l \Lambda(P_m)] \right). \tag{60}
\end{aligned}$$

To finish writing $\overline{\mathcal{F}^2}$ in terms of J we need to find expressions for $\left[\left(\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \right) \Lambda \left(\frac{\mathbb{1}}{D} \right) \right]$ and $\left[\sum_{l,m} \chi_{l,m} P_l \Lambda(P_m) \right]$.

10.1.2 Finding an Expression for $\left[\left(\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \right) \Lambda \left(\frac{\mathbb{1}}{D} \right) \right]$

Since $J = \sum_{l,m} \chi_{l,m} (P_l \otimes \mathbb{1}) \sigma (P_m \otimes \mathbb{1})$ we have,

$$\begin{aligned}
J\sigma &= \sum_{l,m} \chi_{l,m} (P_l \otimes \mathbb{1}) \sigma (P_m \otimes \mathbb{1}) \sigma = \sum_l \chi_{l,0} (P_l \otimes \mathbb{1}) \sigma \\
&= \frac{1}{D} \sum_{l,i,j} \chi_{l,0} P_l |i\rangle \langle j| \otimes |i\rangle \langle j|. \tag{61}
\end{aligned}$$

Therefore,

$$[J\sigma]^{T_2} = \frac{1}{D} \sum_l \chi_{l,0} P_l \tag{62}$$

where the notation “ $[\cdot]^{T_2}$ ” represents the partial trace with respect to the second subsystem. Analogously, $[\sigma J]^{T_2} = \frac{1}{D} \sum_l \chi_{0,l} P_l$ so that,

$$\left[\left(\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \right) \Lambda \left(\frac{\mathbb{1}}{D} \right) \right] = D \left[[J\sigma + \sigma J]^{T_2} [J]^{T_2} \right]. \tag{63}$$

10.1.3 Finding an Expression for $\left[\sum_{l,m} \chi_{l,m} P_l \Lambda(P_m) \right]$

Noting that $J = \frac{1}{D^2} \sum_k \Lambda(P_k) \otimes P_k^T$ we have,

$$[(P_l \otimes P_m^T) J] = \frac{1}{D^2} \sum_k [P_l \Lambda(P_k)] [P_m^T P_k^T] = \frac{1}{D} [P_l \Lambda(P_m)]. \tag{64}$$

Since $\sum_{l,m} \chi_{l,m} P_l \otimes P_m^T = \sum_k A_k \otimes A_k^*$ we can write,

$$\sum_{l,m} \chi_{l,m} [P_l \Lambda(P_m)] = D \left[\left(\sum_k A_k \otimes A_k^* \right) J \right]. \tag{65}$$

We would like to relate $\sum_k A_k \otimes A_k^*$ to J . The natural matrix representation of Λ in the standard basis for $L(\mathbb{C}^D)$, denoted $\Lambda_{ij,kl}^{L(\mathbb{C}^D)}$ is given by,

$$\Lambda_{ij,kl}^{L(\mathbb{C}^D)} = [(|i\rangle\langle j|)^\dagger \Lambda (|k\rangle\langle l|)] = \langle i|\Lambda (|k\rangle\langle l|) |j\rangle. \quad (66)$$

Hence,

$$\begin{aligned} \Lambda_{ij,kl}^{L(\mathbb{C}^D)} &= \langle i| \left(\sum_m A_m |k\rangle\langle l| A_m^\dagger \right) |j\rangle = \sum_m [A_m |k\rangle\langle i|] [A_m^* |l\rangle\langle j|] \\ &= \sum_m \langle i| \otimes \langle j| (A_m \otimes A_m^*) |k\rangle \otimes |l\rangle \\ &= \left(\sum_m A_m \otimes A_m^* \right)_{ij,kl}^{\mathcal{H} \otimes \mathcal{H}} \end{aligned} \quad (67)$$

where $(\sum_m A_m \otimes A_m^*)_{ij,kl}^{\mathcal{H} \otimes \mathcal{H}}$ is the matrix representation of $\sum_m A_m \otimes A_m^*$ in the standard basis for $\mathcal{H} \otimes \mathcal{H}$.

J in the standard basis for $\mathcal{H} \otimes \mathcal{H}$ is,

$$\begin{aligned} J_{ij,kl}^{\mathcal{H} \otimes \mathcal{H}} &= \frac{1}{D} \langle i| \otimes \langle j| \left(\sum_{a,b} \Lambda (|a\rangle\langle b|) \otimes |a\rangle\langle b| \right) |k\rangle \otimes |l\rangle \\ &= \frac{1}{D} \Lambda_{ik,jl}^{L(\mathbb{C}^D)}. \end{aligned} \quad (68)$$

Hence,

$$\left(\sum_m A_m \otimes A_m^* \right)_{ij,pq}^{\mathcal{H} \otimes \mathcal{H}} = \Lambda_{ij,pq}^{L(\mathbb{C}^D)} = D J_{ip,qj}^{\mathcal{H} \otimes \mathcal{H}}. \quad (69)$$

This gives,

$$\begin{aligned} \left[\left(\sum_m A_m \otimes A_m^* \right) J \right] &= \sum_{i,j} \sum_{p,q} \left(\sum_m A_m \otimes A_m^* \right)_{ij,pq}^{\mathcal{H} \otimes \mathcal{H}} J_{pq,ij}^{\mathcal{H} \otimes \mathcal{H}} \\ &= D \sum_{i,j} \sum_{p,q} J_{ip,qj}^{\mathcal{H} \otimes \mathcal{H}} J_{pq,ij}^{\mathcal{H} \otimes \mathcal{H}} \\ &= D \sum_{i,j} \sum_{p,q} (\langle i| \otimes \langle p| J |j\rangle \otimes |q\rangle) (\langle p| \otimes \langle q| J |i\rangle \otimes |j\rangle) \\ &= D \sum_{j,p} [(\mathbb{1} \otimes |j\rangle\langle p|) J (|j\rangle\langle p| \otimes \mathbb{1}) J] \end{aligned} \quad (70)$$

Using the SWAP operation we can write,

$$\left[\left(\sum_m A_m \otimes A_m^* \right) J \right] = D \sum_{j,p} [SWAP(|j\rangle\langle p| \otimes \mathbb{1}) J (|j\rangle\langle p| \otimes \mathbb{1}) J]. \quad (71)$$

The unitary Kraus operator for SWAP, denoted by S , is

$$S = \sum_{i,j=0,\dots,D-1} |i\rangle\langle j| \otimes |j\rangle\langle i|. \quad (72)$$

as is easily verified by noting that $\forall k, l \in \{0, \dots, D-1\}$, $|k\rangle \otimes |l\rangle \mapsto |l\rangle \otimes |k\rangle$. Note that $S = S^\dagger$ and $SS^\dagger = S^2 = \mathbb{1}$. Since

$$\sigma = \frac{1}{D} \sum_{i,j=0,\dots,D-1} |i\rangle\langle j| \otimes |i\rangle\langle j| \quad (73)$$

we have

$$S = D\sigma^{T_1} = D\sigma^{T_2} \quad (74)$$

The partial transpose operation on the first subsystem of a state κ , denoted κ^{T_1} , is given by,

$$\kappa^{T_1} = \sum_{k,l=0,\dots,D-1} (|k\rangle\langle l| \otimes \mathbb{1}) \kappa (|k\rangle\langle l| \otimes \mathbb{1}) \quad (75)$$

with an analogous expression for the partial transpose on the second subsystem. Therefore,

$$\begin{aligned} \left[\left(\sum_m A_m \otimes A_m^* \right) J \right] &= D \sum_{j,p} [S (|j\rangle\langle p| \otimes \mathbb{1}) S J (|j\rangle\langle p| \otimes \mathbb{1}) J] \\ &= D [(SJ)^\dagger (SJ)^{T_1}] \\ &= D^3 [(\sigma^{T_1} J)^\dagger (\sigma^{T_1} J)^{T_1}] \end{aligned} \quad (76)$$

and so,

$$\begin{aligned} \sum_{l,m} \chi_{l,m} [P_l \Lambda(P_m)] &= D \left[\sum_k A_k \otimes A_k^* J \right] = D^4 [(\sigma^{T_1} J)^\dagger (\sigma^{T_1} J)^{T_1}] \\ &= D^4 [(J\sigma^{T_2})^\dagger (J\sigma^{T_2})^{T_2}]. \end{aligned} \quad (77)$$

Hence in total for $\overline{\mathcal{F}^2}$ we have,

$$\begin{aligned}
\overline{\mathcal{F}^2} &= \frac{1}{D^4 + 6D^3 + 11D^2 + 6D} \left([J\sigma]^2 D^4 + D^3 (2[J^2\sigma] + [JJ^T\sigma] + [J^T J\sigma] + 2[J\sigma]) \right. \\
&\quad + D^2 \left(4[J\sigma] + [JJ^T] + 2D [[J\sigma + \sigma J]^{T_2} [J]^{T_2}] + [J^2] \right. \\
&\quad \left. \left. + 1 + [([J]^{T_2})^2] \right) + 3D + 2D^4 [(J\sigma^{T_2})^\dagger (J\sigma^{T_2})^{T_2}] \right). \tag{78}
\end{aligned}$$

10.2 Calculating the Variance for a Single Qubit

In this section $\overline{\mathcal{F}^2} - \overline{\mathcal{F}}^2$ is calculated in a more compact form for the case of a single qubit. Since we already have a simple expression for \mathcal{F} given by (24) we only need to calculate $\overline{\mathcal{F}^2}$. Instead of using (31), we will use (29) which will allow us to group particular terms together to obtain a more simple expression.

To begin, we state some simple facts regarding the χ -matrix. First, the χ -matrix is positive and has trace equal to 1. Second, $\sum_{l,m} \chi_{l,m} P_l P_m = \Lambda(\mathbb{1}) = D\Lambda\left(\frac{\mathbb{1}}{D}\right)$ and third, $\sum_{l,m} \chi_{l,m} P_m P_l = \mathbb{1}$ from trace preservation. The 24 terms in (29) are sorted into groups of 3 each of which is dealt with separately. Since we are working with a single qubit, $D = 2$ in all expressions below. While we do not substitute for D until the end of the calculations, it should be noted that many of the expressions below only hold in the case $D = 2$.

10.2.1 First Group of Terms

The first group consists of the following 10 terms:

$$\begin{aligned}
&\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l][P_m][P_n][P_r] + [P_l P_r][P_m][P_n] + [P_m P_r][P_l][P_n] + [P_l][P_m][P_n P_r] + [P_l P_n][P_m][P_r] \\
&\quad + [P_l P_n][P_m P_r] + [P_m P_n][P_l][P_r] + [P_m P_n][P_l P_r] + [P_l P_m][P_n][P_r] + [P_l P_m][P_n P_r]). \tag{79}
\end{aligned}$$

Using the above properties one can obtain that this group equals,

$$\begin{aligned}
&\chi_{0,0}^2 D^4 + \sum_l \chi_{l,0} \chi_{0,l} D^3 + \sum_l \chi_{0,l}^2 D^3 + \chi_{0,0} D^3 + \sum_l \chi_{l,0}^2 D^3 \\
&+ \sum_{l,m} \chi_{l,m}^2 D^2 + \sum_m \chi_{0,m} \chi_{m,0} D^3 + \sum_{l,m} \chi_{l,m} \chi_{m,l} D^2 + \chi_{0,0} D^3 + D^2. \tag{80}
\end{aligned}$$

10.2.2 Second Group of Terms

The second group consists of the 8 terms

$$\begin{aligned}
&\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_r P_n][P_m] + [P_l P_n P_r][P_m] + [P_m P_r P_n][P_l] + [P_m P_n P_r][P_l] \\
&\quad + [P_r P_m P_l][P_n] + [P_r P_l P_m][P_n] + [P_n P_m P_l][P_r] + [P_n P_l P_m][P_r]). \tag{81}
\end{aligned}$$

These 8 terms are grouped by two and the resulting four sums are calculated independently. For the first sum we deal with five cases:

Case 1: $n \neq r$, $n \neq 0$, and $r \neq 0$. This implies $P_n P_r = -P_r P_n$ and so the above is 0.

Case 2: $n = r$. We get $2 \sum_{l,m,n} \chi_{l,m} \chi_{n,n} [P_l][P_m]$ which equals $2\chi_{0,0} D^2$.

Case 3: $n = 0$. We get, $2 \sum_{l,m,r} \chi_{l,m} \chi_{0,r} [P_l P_r][P_m]$ which is just $2 \sum_l \chi_{l,0} \chi_{0,l} D^2$.

Case 4: $r = 0$. Similarly to case 3 we get $2 \sum_l \chi_{l,0}^2 D^2$.

Case 5: $r = 0$ and $n = 0$. This case is required because we have over-counted for this case twice above. The result is $2\chi_{0,0}^2 D^2$.

Hence the five cases give in total,

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_r P_n][P_m] + [P_l P_n P_r][P_m]) = 2\chi_{0,0} D^2 + 2 \sum_l \chi_{l,0} \chi_{0,l} D^2 + 2 \sum_l \chi_{l,0}^2 D^2 - 4\chi_{0,0}^2 D^2. \quad (82)$$

The other three sums are calculated in a similar fashion and in total we end up with,

$$8\chi_{0,0} D^2 + 8 \sum_l \chi_{l,0} \chi_{0,l} D^2 + 4 \sum_l \chi_{0,l}^2 D^2 + 4 \sum_l \chi_{l,0}^2 D^2 - 16\chi_{0,0}^2 D^2. \quad (83)$$

Substituting $D = 2$ and collecting terms for both the first and second group of terms gives,

$$-48\chi_{0,0}^2 + 48\chi_{1,0} + 32 \sum_l \chi_{0,l}^2 + 16 \sum_l \chi_{l,0}^2 + 16 \sum_l \chi_{l,0} \chi_{0,l} + 4 \sum_{l,m} \chi_{l,m}^2 + 4 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 4 \quad (84)$$

10.2.3 Third Group of Terms

Lastly we have the 6 terms

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_r P_n P_m] + [P_l P_n P_m P_r] + [P_l P_n P_r P_m] + [P_l P_r P_m P_n] + [P_l P_m P_r P_n] + [P_l P_m P_n P_r]) \quad (85)$$

which we group into three pairs as, $\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_r P_n P_m] + [P_l P_r P_m P_n])$, $\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_n P_m P_r] + [P_l P_m P_n P_r])$, and $\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_m P_r P_n] + [P_l P_n P_r P_m])$.

The first pair is easy to calculate using the same cases as above for m and n . The result is,

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_r P_n P_m] + [P_l P_r P_m P_n]) = 4 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 8\chi_{0,0} - 8 \sum_l \chi_{l,0} \chi_{0,l}. \quad (86)$$

The second pair requires a bit more effort and we go through the cases separately,

Case 1: $m \neq n$, $m \neq 0$ and $n \neq 0$. This case gives 0.

Case 2: $m = n$. We get $4 \sum_{l,m} \chi_{l,m} \chi_{m,l}$.

Case 3: $m = 0$. We obtain $2 \sum_{l,n,r} \chi_{l,1} \chi_{n,r} [P_l P_n P_r]$ and after a direct calculation we get

$$4(\chi_{0,0} + \chi_{1,0}(\chi_{0,1} + \chi_{1,0} + i\chi_{2,3} - i\chi_{3,2}) + \chi_{2,0}(\chi_{0,2} + \chi_{2,0} - i\chi_{1,3} + i\chi_{3,1}) + \chi_{3,0}(\chi_{0,3} + \chi_{3,0} + i\chi_{1,2} - i\chi_{2,1})).$$

Case 4: $n = 0$ Similar to case 3 we obtain,

$$4(\chi_{0,0} + \chi_{0,1}(\chi_{0,1} + \chi_{1,0} + i\chi_{2,3} - i\chi_{3,2}) + \chi_{0,2}(\chi_{0,2} + \chi_{2,0} - i\chi_{1,3} + i\chi_{3,1}) + \chi_{0,3}(\chi_{0,3} + \chi_{3,0} + i\chi_{1,2} - i\chi_{2,1})).$$

Case 5: $m = 0$ and $n = 0$. We obtain $4 \sum_l \chi_{l,0} \chi_{0,l}$.

Combining the 5 cases gives,

$$\begin{aligned} \sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_n P_m P_r] + [P_l P_m P_n P_r]) &= 4 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 8\chi_{0,0} \\ &+ 4(\chi_{0,1} + \chi_{1,0})(\chi_{0,1} + \chi_{1,0} + i(\chi_{2,3} - \chi_{3,2})) + 4(\chi_{0,2} + \chi_{2,0})(\chi_{0,2} + \chi_{2,0} + i(\chi_{3,1} - \chi_{1,3})) \\ &+ 4(\chi_{0,3} + \chi_{3,0})(\chi_{0,3} + \chi_{3,0} + i(\chi_{1,2} - \chi_{2,1})) - 8 \sum_l \chi_{0,l} \chi_{l,0} \end{aligned}$$

For the third pair we have,

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_m P_r P_n] + [P_l P_n P_r P_m]) = [\Lambda^\dagger (\Lambda^\dagger (\mathbb{1}))] + [\Lambda (\Lambda (\mathbb{1}))] = 4. \quad (87)$$

and so combining the three pairs gives,

$$\begin{aligned} &8 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 16\chi_{0,0} - 16 \sum_l \chi_{l,0} \chi_{0,l} + 4 + 4(\chi_{0,1} + \chi_{1,0})(\chi_{0,1} + \chi_{1,0} + i(\chi_{2,3} - \chi_{3,2})) \\ &+ 4(\chi_{0,2} + \chi_{2,0})(\chi_{0,2} + \chi_{2,0} + i(\chi_{3,1} - \chi_{1,3})) + 4(\chi_{0,3} + \chi_{3,0})(\chi_{0,3} + \chi_{3,0} + i(\chi_{1,2} - \chi_{2,1})). \quad (88) \end{aligned}$$

We can calculate another expression for the three pairs by noting that four of the terms give,

$$[\Lambda (\Lambda^\dagger (\mathbb{1}))] + [\Lambda^\dagger (\Lambda (\mathbb{1}))] + [\Lambda (\Lambda (\mathbb{1}))] + [\Lambda^\dagger (\Lambda^\dagger (\mathbb{1}))] = 3D + [\Lambda^\dagger (\Lambda (\mathbb{1}))] = 6 + [\Lambda (\mathbb{1})^2] \quad (89)$$

with the remaining two terms, $\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} [P_l P_n P_m P_r]$ and $\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} [P_l P_r P_m P_n]$, being complex conjugates of one another. From the calculation of the first pair given above we have,

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} ([P_l P_r P_n P_m] + [P_l P_r P_m P_n]) = 4 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 8\chi_{1,1} - 8 \sum_l \chi_{l,1} \chi_{1,l} \quad (90)$$

and since $\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} [P_l P_r P_n P_m] = 2$ we get,

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} [P_l P_r P_m P_n] = \sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} [P_l P_r P_m P_n] = 4 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 8 \chi_{0,0} - 8 \sum_l \chi_{l,0} \chi_{0,l} - 2. \quad (91)$$

Therefore the three pairs can also be written as,

$$2 + \left[\Lambda(\mathbb{1})^2 \right] + 8 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 16 \chi_{0,0} - 16 \sum_l \chi_{l,0} \chi_{0,l} \quad (92)$$

where,

$$\begin{aligned} \left[\Lambda(\mathbb{1})^2 \right] &= 2 + 4(\chi_{0,1} + \chi_{1,0})(\chi_{0,1} + \chi_{1,0} + i(\chi_{2,3} - \chi_{3,2})) + 4(\chi_{0,2} + \chi_{2,0})(\chi_{0,2} + \chi_{2,0} + i(\chi_{3,1} - \chi_{1,3})) \\ &\quad + 4(\chi_{0,3} + \chi_{3,0})(\chi_{0,3} + \chi_{3,0} + i(\chi_{1,2} - \chi_{2,1})). \end{aligned} \quad (93)$$

Combining all 24 terms and noting $[\pi_{\text{sym}}(4, D)] = \frac{120}{24}$ we obtain,

$$\overline{\mathcal{F}^2} = \frac{\left(-48\chi_{0,0}^2 + 64\chi_{0,0} + 16(\chi\chi^T + \chi^T\chi)_{0,0} + 16(\chi^2)_{0,0} + 4[\chi\chi^T] + 12[\chi^2] + 8 + \left[\Lambda(\mathbb{1})^2 \right] \right)}{120}. \quad (94)$$

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