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 an explicit basis-independent expression for its variance which can be extended to calculate all higher order moments. Using these results we obtain a simple expression for the variance of a single qubit system and deduce the asymptotic behavior for large-dimensional quantum systems. Applications of these results to quantum chaos and randomized benchmarking are discussed.
I. INTRODUCTION

The building blocks of a quantum computation are quantum logic gates, unitary operations that are applied in a specific sequence to the physical systems that encode quantum information. In theory, any quantum algorithm can be implemented with high precision by applying a correctly chosen sequence of gates – but in practice, gates have errors. In real experiments, we attempt to apply an ideal gate $U$, but what really happens is a noisy quantum operation $E$. If we want to end up with a dynamical evolution close to the desired algorithm, $E$ had better be “close” to $U$.

How close $E$ is to $U$, operationally, depends on the state of the system they act on. Some states may evolve identically under $E$ and $U$, while for other states they produce drastically different outputs! Understanding quantum noise and designing error-resistant devices requires state-independent characterizations of the noise. One way to get such a quantity, beginning with a state-dependent gate fidelity $F(\rho)$, is to average it over all [pure] input states. This average gate fidelity, $F$, provides a concise, useful measure of error.

However, it provides no information about fluctuations in the gate fidelity – i.e., how the error varies over input states. The magnitude of the fluctuations is a useful diagnostic. It provides information about the worst-case fidelity, which is relevant for fault-tolerant design. Large fluctuations also suggest that the average error may be dominated by a few very error-prone states, in which case addressing those states can produce dramatic improvements in average fidelity. Large fluctuations may also indicate hidden high-fidelity information-preserving structures such as pointer bases or decoherence-free subspaces [1].

In this paper, we calculate the variance of the gate fidelity analytically, and discuss how it might be measured in experiments (and challenges to doing so!). Moreover, we develop a general method for calculating higher moments of the gate fidelity, which can be applied to other purposes. This problem has been considered before: Ref. [2] solved the special case where $E$ maps pure states into pure states. Our calculation applies to general quantum operations. We apply it to a couple of interesting specific cases: operations acting on a single qubit, and on very large ($\dim(H) \to \infty$) systems.

We begin, in Section II, by introducing the framework and formulae that we will use. In Section III A we calculate the average gate fidelity as a warm-up, and confirm agreement with previous calculations. We then calculate the variance in Section III B and briefly discuss higher order moments in Section IV. Finally, we calculate explicit expressions for gates on a single qubit and asymptotically large systems (Section V). We conclude, in Section VI, by discussing applications to randomized noise characterization, and to estimating fidelity decay under controlled perturbations of chaotic systems.
II. BACKGROUND

Before beginning, we set some notation for the rest of the paper. $\mathcal{H}$ represents a system’s Hilbert space, assumed in this paper to be of finite dimension $d$. $L(\mathcal{H})$ is the set of all linear operators on $\mathcal{H}$ (i.e., $d \times d$ matrices), and $\mathcal{D}(\mathcal{H})$ is the set of (mixed) quantum states on $\mathcal{H}$, containing all the positive, trace-1 operators in $L(\mathcal{H})$. Pure states are represented by projectors $|\psi\rangle\langle\psi|$ in the complex projective space $\mathbb{C}P^{d-1}$.

A. Quantum Operations

Quantum operations – a.k.a. processes or channels – describe the dynamical evolution of quantum systems over a period of time. These dynamics may be reversible or irreversible, and they may even involve adding or discarding parts of the system, so the initial and final Hilbert spaces need not be identical. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces of dimension $d_1$ and $d_2$, representing (respectively) the input and the output of a quantum dynamical process. We will denote the set of all linear (super)operators from $L(\mathcal{H}_1)$ to $L(\mathcal{H}_2)$ by $\mathcal{T}(\mathcal{H}_1, \mathcal{H}_2)$, and if $\mathcal{H}_1 = \mathcal{H} = \mathcal{H}_2$, denote it $\mathcal{T}(\mathcal{H})$.

Not every linear superoperator $E$ is a valid quantum operation. First, $E$ must preserve the trace of the input state $\rho_1 \in \mathcal{D}(\mathcal{H}_1)$, for it represents total probability. Furthermore, a superoperator $E$ that maps some positive semidefinite $\rho_1 \geq 0$ to a non-positive operator is physically impossible – it is not a positive map. In fact, to represent a valid operation, a superoperator must satisfy the even stronger condition of complete positivity: given an ancillary system represented by a Hilbert space $\mathcal{A}$, $E$ must map every joint state $\rho_{\mathcal{H}_1, \mathcal{A}} \in \mathcal{D}(\mathcal{H}_1 \otimes \mathcal{A})$ to a positive semidefinite state of $\mathcal{H}_2 \otimes \mathcal{A}$. Complete positivity is both necessary and sufficient (together with trace-preservingness) for $E$ to represent a valid physical process, so we will restrict our focus to these CPTP linear maps.

There are various useful ways of representing a CPTP map $E$ (see Ref. [3] for more details). The most brutally straightforward one comes from the observation that $L(\mathcal{H})$ is itself a Hilbert space of dimension $d^2$ under the Hilbert-Schmidt inner product,

$$\langle A | B \rangle \equiv \text{tr} \left( A^\dagger B \right).$$

Let $\{B_i\}$ be any orthogonal basis for $L(\mathcal{H})$ with the normalization condition $\text{tr} \left( B_i^\dagger B_j \right) = d$. This choice of normalization, while nonstandard, is convenient for a variety of reasons – e.g., it allows the basis matrices to be unitary.
Using such basis, $E$ can be written as a $d^2 \times d^2$ matrix with coefficients

$$E_{ij} = \frac{(B_i | E | B_j)}{\sqrt{(B_i | B_i) (B_j | B_j)}} = \frac{\text{tr} (B_i^\dagger E(B_j))}{d}. $$

The generalization to maps with different input and output spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ should be obvious.

While this representation is useful and straightforward, it can represent any linear map on $L(\mathcal{H})$. Complete positivity is neither mandated nor easily tested in this representation. So we turn to the Choi-Jamiolkowski representation. As before, let $\{B_i\}$ be an orthogonal basis for $L(\mathcal{H})$. Now let $\chi$ be a $d^2 \times d^2$ matrix of coefficients and define

$$E(\rho) = \sum_{i,j} \chi_{ij} B_i \rho B_j^\dagger. $$

Like the standard representation given above, this “$\chi$-matrix” representation is capable of representing any linear map on $L(\mathcal{H})$. (This is easily proven by choosing a basis consisting of the normalized matrix units $\{\sqrt{d}|k\rangle \langle l| : k, l = 1 \ldots d\}$. ) However, $E$ is completely positive if and only if $\chi$ is positive semidefinite! This statement is basis-independent; changing $\{B_i\}$ corresponds to a unitary transformation of $\chi$. If $\chi$ is positive semidefinite, then it can be diagonalized, and $E$ can be written as

$$E(\rho) = \sum_i K_i \rho K_i^\dagger. $$

(1)

This is the Kraus form, or operator-sum representation, of $E$. Any linear map of the form given in Eq. (1) is completely positive (even when the $\{K_i\}$ are not orthogonal), and every CP map can be written this way.

To actually construct $\chi$ from a given $E$, we consider an augmented Hilbert space $\mathcal{H} \otimes \mathcal{H}$. Let $|\Psi\rangle$ be the symmetric maximally entangled ( “Bell”) state,

$$|\Psi\rangle = \frac{1}{\sqrt{d}} \sum_{a=1}^d |a\rangle \otimes |a\rangle, $$

and define the Jamiolkowski state of $E$ as the Choi matrix of $E$ scaled by a factor $d$,

$$\rho_J = (E \otimes \mathbb{1}) |\Psi\rangle \langle \Psi| = \frac{1}{d} \sum_{a,b=1}^d E(|a\rangle \langle b|) \otimes |a\rangle \langle b|. $$

It is easy to show by direct calculation that the elements of $\rho_J$, in the standard basis $\{|k\rangle \otimes |l\rangle\}$, are identical to the elements of the $\chi$ matrix in the supernormalized basis of matrix units $\{B_{kl} = \sqrt{d}|k\rangle \langle l|\}$!

$$\chi_{ij,kl} = (\rho_J)_{ij,kl}. $$

So, although $\chi$ and $\rho_J$ act on different vector spaces, the spaces and the matrices themselves are isomorphic. Thus, $\chi$ and $\rho_J$ are merely different aspects of a single Choi-Jamiolkowski representation. We will use $\chi$ for both in the remainder of this paper.
B. The Choi-Jamiolkowski isomorphism; partial traces, partial transposes, and notation

The power and utility of the Choi-Jamiolkowski representation are due in large part to the fact that it establishes an isomorphism between (on the one hand) completely positive maps on $L(\mathcal{H})$, and (on the other hand) a certain class of bipartite states on $\mathcal{H} \otimes \mathcal{H}$. The states in question are those where the state of the second, ancillary system ($\rho_2$) is maximally mixed, for the Jamiolkowski state is produced by applying $E \otimes \mathbb{I}$ to a maximally entangled state. Since $\rho_2$ is initially maximally mixed, and the map only acts on the first system, the Jamiolkowski state must also have $\rho_2 = \mathbb{I}/d$.

We will make extensive use of the Jamiolkowski representation. So a channel $E$ will be represented by a matrix $\chi$, which generally is interpreted as a bipartite density matrix. Two important operations on such a state are:

- The partial trace over one subsystem. For any bipartite matrix $A$, we will denote the partial trace over subsystem $i$ by $\text{tr}_i[A]$. When the partial trace is applied to a state, it generates the reduced density matrix of the remaining subsystem: $\rho_2 = \text{tr}_1 \rho$.

- The partial transpose over one subsystem. For any bipartite matrix $A$, we will denote the partial transpose of $A$ with respect to the $i$th subsystem by $A^{T_i}$. (Similarly, $A^T$ indicate the full transpose of $A$, with respect to both subsystems). Partial transposition is not a completely positive operation; in particular, it transforms many entangled states into negative matrices. Interestingly, it appears naturally in our result. An explicit formula for the partial transpose is given by:

$$A^{T_1} = \sum_{k,l=0}^{d-1} (|k\rangle \langle l| \otimes \mathbb{I}) A (|k\rangle \langle l| \otimes \mathbb{I})$$

$$A^{T_2} = \sum_{k,l=0}^{d-1} (\mathbb{I} \otimes |k\rangle \langle l|) A (\mathbb{I} \otimes |k\rangle \langle l|).$$

We will also use the Choi-Jamiolkowski isomorphism occasionally. Its primary function is to associate bipartite states with superoperators, but the isomorphism extends to other objects in the relevant vector spaces – in particular, bases. We will find it essential for some calculations to write a channel’s $\chi$-matrix in specific bases: this will either be a basis for $L(\mathcal{H})$, or a basis for $\mathcal{H} \otimes \mathcal{H}$. The isomorphism is as follows: If $\{P_k\}$ is a basis for $L(\mathcal{H})$, then define $|\psi_k\rangle = P_k \otimes \mathbb{I} |\Psi\rangle$, and $\{|\psi_k\rangle\}$ is the corresponding basis for $\mathcal{H} \otimes \mathcal{H}$. Choosing a basis in this way ensures that $\chi$ is entry-wise identical in the two representations.
C. Generalized Pauli and Bell bases

For qubits \((d = 2)\), the Pauli operators are an exceptionally convenient basis for \(L(\mathcal{H})\). The corresponding basis of bipartite states is the Bell basis. In higher dimensions, it’s generally not possible to pick a basis with all the nice properties of the Pauli operators, but we can generalize most of them.

When necessary in our calculations, we will make use of a hermitian, orthogonal, supernormalized basis of matrices \(\{P_a\}\) satisfying the following conditions:

\[
\begin{align*}
\text{tr} (P_a P_b) &= d \delta_{a,b} \\
P_a^\dagger &= P_a \\
P_0 &= \mathbb{1}.
\end{align*}
\]

In dimension \(d = 2\), the ubiquitous Pauli operators form such a basis; in higher dimensions, the generalized Gell-Mann operators \([4]\) satisfy the conditions. We require only the listed conditions — most importantly, the fact that \(P_0 = \mathbb{1}\) and therefore every other \(P_k\) is traceless, which singles out the \(\chi_{0,0}\) matrix element as a unitary invariant of \(\mathcal{E}\) — so we will not specify a particular basis. The corresponding basis of bipartite states is orthonormal, and because \(P_0 = \mathbb{1}\), we have \(|\psi_0\rangle = |\Psi\rangle\). We will refer to this basis as the “generalized Bell basis,” though it does not by any means generalize all the properties of the Bell states.

Finally, we will make extensive use of the bipartite projector

\[
\chi_0 = |\psi_0\rangle\langle \psi_0| = |\Psi\rangle\langle \Psi|.
\]

It is the \(\chi\) representation of the identity channel \(\mathcal{E} = \mathbb{1}\), which motivates the notation \(\chi_0\). Moreover, it enables us to write basis-specific expressions in a basis-invariant way — e.g., the unitary invariant \(\chi_{0,0}\) mentioned above can be written in a basis-invariant way as

\[
\chi_{0,0} = \langle \psi_0 | \chi | \psi_0 \rangle = \text{tr} [\chi \chi_0].
\]

D. Gate Fidelity

Suppose that \(U\) is a unitary quantum operation (i.e., \(U(\rho) = U \rho U^\dagger\) for some unitary \(U\)), and \(\mathcal{E}\) is a noisy implementation of \(U\). Then the gate fidelity between \(\mathcal{E}\) and \(U\), given state \(\rho\), is

\[
\mathcal{F}_{\mathcal{E},U}(\rho) = \left( \text{tr} \sqrt{\sqrt{\mathcal{E}(\rho)} U(\rho) \sqrt{\mathcal{E}(\rho)}} \right)^2.
\]
It is simply the state fidelity between $E(\rho)$ and $U(\rho)$, defined in general as

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

Fidelity measures indistinguishability: $F = 1$ means the states are identical, while $F = 0$ implies that a single measurement can distinguish them perfectly. Thus, the gate fidelity $F_{E,U}(\rho)$ is a convenient measure of how distinguishable the actions of $U$ and $E$ are – on the state $\rho$.

If the input state is pure (so $\rho = |\phi\rangle \langle \phi|$), then

$$F_{E,U}(\phi) = \text{tr} \left[ U |\phi\rangle \langle \phi| \right] E (|\phi\rangle \langle \phi|) \right].$$

If $\{K_k\}$ are Kraus operators for $E$, then we can rewrite this using the cyclic property of the trace as

$$F_{E,U}(\phi) = \text{tr} \left[ U |\phi\rangle \langle \phi| U^\dagger \sum_k K_k |\phi\rangle \langle \phi| K_k^\dagger \right] = \text{tr} \left[ |\phi\rangle \langle \phi| U^\dagger \circ E(|\phi\rangle \langle \phi|) \right] = \text{tr} \left[ |\phi\rangle \langle \phi| \Lambda(|\phi\rangle \langle \phi|) \right]$$

where $\Lambda = U^\dagger \circ E$ represents how much $E$ deviates from $U$.

We would like a performance measure that removes the state dependence – an invariant property of the gate fidelity’s distribution. If we focus our attention on pure input states, then this distribution is well defined, for the set of pure quantum states, $\mathbb{C}P^{d-1}$, admits a unique (and natural) invariant distribution. It is the Fubini-Study (FS) measure which we will denote by $\mu_{FS}$. This is the Borel measure induced by the Fubini-Study metric on $\mathbb{C}P^{d-1}$, and also the unitarily invariant Haar measure on $\mathbb{C}P^{d-1}$. The average fidelity under $\mu_{FS}$ has been derived previously (see, e.g., Refs. [6, 7]), and we will derive it again in Section III as a warmup for computing higher moments of the gate fidelity distribution.

### E. Permutation Operators and the Symmetric Subspace

We are trying to compute averages over a unitarily invariant measure, and therefore over the unitary group itself. To do so, we will begin by transforming polynomial functions of degree $k$ into linear functions on $k$ copies of the Hilbert space in question. We will then rely on a simple and beautiful result called Schur-Weyl duality, which states (in essence) that the actions of the unitary group and the permutation group (on such a $k$-fold tensor product) commute, and their irreducible representations (irreps) share a set of labels. Rather than discuss Schur-Weyl duality in detail, we will only introduce the tools that we need. In this section, we will briefly discuss permutation operators, the symmetric group, the totally symmetric subspace of $\mathcal{H}^\otimes k$, and a couple of technical results that will be useful later.
Let $\mathcal{H}$ be a Hilbert space and $\mathcal{H}^\otimes k$ a tensor product of $k$ copies of it. If $S_k$ is the symmetric group on $k$ objects and $\sigma \in S_k$ is a permutation, then there exists a unitary operator $P_\sigma$ that implements $\sigma$ on $\mathcal{H}^\otimes k$:

$$P_\sigma (|\psi_1\rangle \otimes \cdots \otimes |\psi_k\rangle) = |\psi_{\sigma^{-1}(1)}\rangle \otimes \cdots \otimes |\psi_{\sigma^{-1}(k)}\rangle.$$ 

The totally symmetric subspace of $\mathcal{H}^\otimes k$ comprises all the states that are invariant under every such permutation operator – or, to put it another way, it is the intersection of the +1 eigenspaces of all $P_\sigma$. The projector onto this space is given by

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

This projector appears in integrals over the unitary group, for the following reason (see Ref. [8]). Suppose we take a state $|\psi\rangle \in \mathcal{H}$, and then construct the projector onto its $k$-fold tensor product, $|\psi\rangle (|\psi\rangle^\otimes k)$. This projector is a +1 eigenoperator of every permutation, so it lies in the totally symmetric subspace. Now, if we take the average of all such projectors according to the unitarily invariant measure $\mu_{FS}$ (denoted $|\psi\rangle (|\psi\rangle^\otimes k)$), then we get an operator in $L(\mathcal{H}^\otimes k)$ that: (i) is invariant under all unitaries $U^\otimes k$; (ii) is supported on the totally symmetric subspace; and (iii) has unit trace. By Schur’s Lemma, a unitarily invariant operator is a weighted sum of projectors onto irreducible representations of the unitary group. The only such operators supported on the totally symmetric subspace are proportional to $\pi_{\text{sym}}$ itself. Since $|\psi\rangle (|\psi\rangle^\otimes k)$ has unit trace,

$$\frac{|\psi\rangle (|\psi\rangle^\otimes k)}{\text{tr}[|\psi\rangle (|\psi\rangle^\otimes k)]} = \int_{\psi \in CP^{d-1}} |\psi\rangle (|\psi\rangle^\otimes k)d\mu_{FS} = \frac{\pi_{\text{sym}}(k,d)}{\text{tr}[\pi_{\text{sym}}(k,d)]}.$$ 

The normalization constant is easy to evaluate by counting arguments. The symmetric subspace of $\mathcal{H}^\otimes k$ is spanned by the bosonic Fock states, $|n_1,n_2,\ldots,n_d\rangle$, which are indexed by the number of particles $n_i$ in state $i$, subject to $\sum_i n_i = k$. Counting such states, we get

$$\text{tr}[\pi_{\text{sym}}(k,d)] = \left(\begin{array}{c}k+d-1 \\ d-1\end{array}\right) = \frac{d(d+1)(d+2)\ldots(d+k-1)}{k!}.$$ 

Suppose that we have $k$ operators $A_1,\ldots,A_k$ in $L(\mathcal{H})$, and a permutation $\sigma \in S_k$ written as a product of disjoint cycles $(a_1\ldots a_r)\ldots(a_q\ldots a_k)$. Then

$$\text{tr}[(A_1 \otimes \cdots \otimes A_k) P_\sigma] = \text{tr}[A_{a_1}\ldots A_{a_r}] \ldots \text{tr}[A_{a_q}\ldots A_{a_k}].$$ 

So, to calculate $\text{tr}[(A_1 \otimes \cdots \otimes A_k) P_\sigma]$, we can write $\sigma$ in cyclic notation, replace “$\psi$” with operator $A_i$, and replaces each “( )” with “tr[ ]”.

(1)

(2)

(3)

(4)
III. CALCULATING THE VARIANCE OF THE GATE FIDELITY

We can use these tools to rederive the average value of $F_{E,U}$ (hereafter denoted simply by $F$), and also to calculate its variance:

$$\text{Var} (F) = \overline{F^2} - \overline{F}^2.$$ 

Our ultimate goal is a basis-independent expression (Eq. (17)), entirely in terms of the $\chi$ matrix for $\Lambda \equiv U^\dagger \circ E$.

A. Average Fidelity

To determine $\text{Var}(F)$, we need to calculate both $\overline{F}$ and $\overline{F^2}$. Fortunately, the tools in the previous section can be used calculate any moment of $F$, although the calculation of $\overline{F^n}$ gets rapidly harder with increasing $n$. So we begin with $\overline{F}$, which is already well-known [7], as a sort of warmup.

We begin by expanding the state-dependent gate fidelity in terms of $\Lambda$’s Kraus operators $\{K_i\}$,

$$F(\psi) = \text{tr} [\Lambda(\psi)\psi] = \sum_i \text{tr} [K_i \psi] \cdot \text{tr} [\psi^\dagger K_i^\dagger]$$

This expression is a Hilbert-Schmidt inner product between (i) a term including all the Kraus operators, and (ii) a term including all the $\psi$-dependence. To average over $\psi$, we need only average the second term, using Eq. (2):

$$\overline{F} = \int F(\psi) d\psi = \sum_i \text{tr} \left[ \left( K_i \otimes K_i^\dagger \right) P_\sigma \right] = \sum_i \text{tr} \left[ \left( K_i \otimes K_i^\dagger \right) \frac{\pi_{\text{sym}}(2,d)}{\text{tr} \left( \pi_{\text{sym}}(2,d) \right)} \right]. \tag{5}$$

We now expand $\pi_{\text{sym}}(2,d)$ as a sum of permutation operators, invoke Eq. (4) to evaluate the traces, and use Eq. (3) to evaluate the normalization:

$$\overline{F} = \frac{1}{2 \text{tr} \left( \pi_{\text{sym}}(2,d) \right)} \sum_{i} \sum_{\sigma \in S_2} \text{tr} \left[ \left( K_i \otimes K_i^\dagger \right) P_\sigma \right] = \frac{\sum_i \left( \text{tr} [K_i] \text{tr} [K_i^\dagger] \right)}{d^2 + d} + d.$$ 

If we write $\overline{F}$ in terms of the $\chi$ matrix, as $\Lambda(\rho) = \sum_{l,m} \chi_{l,m} P_l P_m$, then the same calculation yields

$$\overline{F} = \frac{2}{d^2 + d} \sum_{l,m} \text{tr} [\chi_{l,m} P_l \otimes P_m \pi_{\text{sym}}(2,d)] = \frac{1}{d^2 + d} \sum_{l,m} \chi_{l,m} \left( \text{tr} [P_l] \text{tr} [P_m] + \text{tr} [P_l P_m] \right) = \frac{\chi_{0,0}d + 1}{d + 1},$$

which agrees with the results from Refs. [6, 7]. We can rewrite this in a basis-invariant fashion by recalling that $\chi_{0,0} = \text{tr} [\chi \chi_0]$, so

$$\overline{F} = \frac{\text{tr} [\chi \chi_0] d + 1}{d + 1}. \tag{6}$$
We observe that $\text{tr} [\chi \chi_0]$ represents the overlap of $\Lambda$ with the identity channel, and therefore how much $\Lambda$ leaves the input state unchanged. It is also a unitary invariant of $\Lambda$: $\chi_{0,0}$ does not change if we rotate $\Lambda$ by a unitary channel $U$, mapping $\Lambda \rightarrow U^{-1} \circ \Lambda \circ U$.

B. Variance of the Fidelity

Now, let’s tackle the calculation of $\mathcal{F}^2$. As done previously, we expand $\mathcal{F}^2$ in terms of $\Lambda$’s Kraus operators,

$$\mathcal{F}^2(|\psi\rangle \langle \psi|) = \text{tr} [\Lambda(|\psi\rangle \langle \psi|) \cdot |\psi\rangle \langle \psi|] = \sum_i \text{tr} [K_i |\psi\rangle \langle \psi|] \sum_j \text{tr} [K_j |\psi\rangle \langle \psi|]$$

and then use Eq. (2) to simplify the average, $\mathcal{F}^2$, as

$$\mathcal{F}^2 = \sum_{i,j} \text{tr} \left[ \left( K_i \otimes K_i^\dagger \otimes K_j \otimes K_j^\dagger \right) \cdot |\psi\rangle \langle \psi|^{\otimes 4} \right],$$

and then use Eq. (2) to simplify the average, $\mathcal{F}^2$, as

$$\mathcal{F}^2 = \sum_{i,j} \text{tr} \left[ \left( K_i \otimes K_i^\dagger \otimes K_j \otimes K_j^\dagger \right) \cdot |\psi\rangle \langle \psi|^{\otimes 4} \right] = \sum_{i,j} \text{tr} \left[ \pi_{\text{sym}}(4, d) \right] \pi_{\text{sym}}(4, d).$$

Finally, we write $\pi_{\text{sym}}(2, d)$ as a sum of permutation operators, invoke Eq. (4) to evaluate the traces, and use Eq. (3) to evaluate the normalization:

$$\mathcal{F}^2 = \sum_{i,j} \text{tr} \left[ \left( K_i \otimes K_i^\dagger \otimes K_j \otimes K_j^\dagger \right) \cdot |\psi\rangle \langle \psi|^{\otimes 4} \right] = \sum_{i,j} \text{tr} \left[ \left( K_i \otimes K_i^\dagger \otimes K_j \otimes K_j^\dagger \right) \cdot |\psi\rangle \langle \psi|^{\otimes 4} \right] = \sum_{i,j} \text{tr} \left[ \pi_{\text{sym}}(4, d) \right] \pi_{\text{sym}}(4, d).$$

There are 24 products of traces in the sum, each corresponding to one of the $4!$ permutations of 4 objects, so the ellipsis in the last equation represents 22 more terms.

In this case, it’s more productive to use the matrix basis $\{P_i\}$ and write $\mathcal{F}$ using the $\chi$ matrix. The same calculation then yields

$$\mathcal{F}^2 = \sum_{i,m,n,r} \chi_{i,m} \chi_{n,r} \left( \text{tr} [P_i] \text{tr} [P_m] \text{tr} [P_n] \text{tr} [P_r] + \text{tr} [P_i P_j] \text{tr} [P_m] \text{tr} [P_n] + ... \right).$$

By writing out all 24 terms in the summation (excluded here for reasons of space and extreme tediousness), we can...
use the properties of the \{P_i\} basis – e.g., \(\text{tr} P_i P_j = d \delta_{ij}\), and \(\text{tr} P_i = d \delta_{i,0}\) – to simplify this expression to

\[
F_2^2 = \frac{1}{d(d+1)(d+2)(d+3)} \left( d^4 \text{tr}[\chi \chi^0]^2 
+ d^3 \text{tr} \left[ \chi_0 \left( 2\chi^2 + \chi \chi^T + \chi^T \chi + 2\chi \right) \right] 
+ d^2 \left( 4\text{tr}[\chi \chi_0] + \text{tr} \left[ \chi \chi^T \right] + \text{tr} \left[ \chi^2 \right] + 1 \right) 
+ d \left( 2 \sum_{i,j} \text{tr} [ (\chi_{i,0} + \chi_{0,i}) P_i \Lambda (\mathbb{1}) ] + 3 \right) 
+ 2 \text{tr} \left[ \sum_{l,m} \chi_{l,m} P_l \Lambda (P_m) \right] + \text{tr} \left[ (\Lambda (\mathbb{1}))^2 \right] \right).
\]  

(10)

All but three of the terms in Eq. (10) are expressed solely in terms of \(\Lambda\)'s \(\chi\)-matrix. The exceptions are:

- \(\text{tr} \left[ (\Lambda (\mathbb{1}))^2 \right]\) comes from 4-cycle permutations like \(\sigma = (1234)\), which produce terms of the form \(\sum_{l,m} \chi_{l,m} \chi_{n,r} \text{tr} [P_l P_m P_n P_r]\).

- \(2d \text{tr} [\sum_i (\chi_{i,0} + \chi_{0,i}) P_i \Lambda (\mathbb{1})]\) comes from 3-cycle permutations like \(\sigma = (123)(4)\), which produce terms of the form \(\sum_{l,m} \chi_{l,m} \chi_{n,r} \text{tr} [P_l P_m P_n P_r]\).

- \(2 \text{tr} \left[ \sum_{l,m} \chi_{l,m} P_l \Lambda (P_m) \right]\) comes from 4-cycle permutations like \(\sigma = (1324)\), which produce terms of the form \(\sum_{l,m} \chi_{l,m} \chi_{n,r} \text{tr} [P_l P_m P_n P_r]\).

Our next order of business is to rewrite these terms in a basis-invariant fashion, using \(\chi, \chi_0\), the partial transpose, and the partial trace (see Section II).

The first term is easy. It’s straightforward to verify that

\[
\Lambda \left( \frac{\mathbb{1}}{d} \right) = \text{tr}_2 \chi,
\]

so

\[
\text{tr} \left[ (\Lambda (\mathbb{1}))^2 \right] = d^2 \text{tr} \left[ (\text{tr}_2 \chi)^2 \right].
\]

(11)

We can rewrite the second term using the non-Hermitian operator

\[
\chi \chi_0 = \sum_{l,m} \chi_{l,m} (P_l \otimes \mathbb{1}) \chi_0 (P_m \otimes \mathbb{1}) \chi_0 = \sum_l \chi_{l,0} (P_l \otimes \mathbb{1}) \chi_0 = \frac{1}{d} \sum_{l,i,j} \chi_{l,0} P_l |i\rangle \langle j| \otimes |i\rangle \langle j|
\]

and its adjoint \(\chi_0 \chi\). Partial tracing over the second (ancillary) system yields

\[
\text{tr}_2 (\chi \chi_0) = \frac{1}{d} \sum_l \chi_{l,0} P_l,
\]

\[
\text{tr}_2 (\chi_0 \chi) = \frac{1}{d} \sum_l \chi_{0,l} P_l,
\]
which provides a basis-invariant expression for the second term:

\[
\text{tr} \left[ \left( \sum_l (\chi_{l,0} + \chi_{0,l}) P_l \right) \Lambda (1) \right] = d^2 \text{tr} \left[ \text{tr}_2 (\chi \chi_0 + \chi_0 \chi) \text{tr}_2 \chi \right].
\]

To rewrite the third exceptional term, we apply a few more tricks. First, we observe that for any bipartite operator \( A \otimes B \),

\[
\text{tr} \left[ \chi^{T_2} (A \otimes B) \right] = \frac{1}{d} \text{tr} \left[ AA(B) \right].
\]

This is easily shown from the definition of \( \chi \). Next, we note that since \( \chi_0 = \frac{1}{d} \sum_{l,m} \chi_{lm} |l\rangle \langle m| \otimes |l\rangle \langle m| \), its partial transpose (over either subsystem) is

\[
\chi_0^{T_1} = \chi_0^{T_2} = \frac{1}{d} \sum_{l,m} |l\rangle \langle m| \otimes |m\rangle \langle l|.
\]

This bipartite operator is proportional to the unitary SWAP gate (which we denote \( S \)), which maps \(|l\rangle \otimes |m\rangle \rightarrow |m\rangle \otimes |l\rangle\).

Now, consider the operator \( S(S\chi)^{T_1} \), which can be written out as:

\[
S(S\chi)^{T_1} = \frac{1}{d} S \left( S \sum_{ijlm} \chi_{lm} P_l |i\rangle \langle j| P_m \otimes |i\rangle \langle j| \right)^{T_1} = \frac{1}{d} S \left( \sum_{ijlm} \chi_{lm} |i\rangle \langle j| P_m \otimes P_l |i\rangle \langle j| \right)^{T_1} = \frac{1}{d} \sum_{ijlm} \chi_{lm} P_l |i\rangle \otimes P_m^{T} |j\rangle \langle j|.
\]

Together, these two observations imply that

\[
\text{tr} \left[ \chi^{T_2} (S(S\chi)^{T_1})^{T_2} \right] = \frac{1}{d^2} \sum_{lm} \chi_{lm} \text{tr}[P_l \Lambda(P_m)],
\]

but \( \text{tr} \left[ X^{T_2} Y^{T_2} \right] = \text{tr} [XY] \) (just as for the full transpose), so the two partial transposes cancel. Substituting in \( S = d\chi_0^{T_1} \), we get a basis-independent expression for the third exceptional term:

\[
\sum_{l,m} \chi_{lm} \text{tr}[P_l \Lambda(P_m)] = d^4 \text{tr} \left[ \chi^{T_1} \chi^{T_1} \right] = d^4 \text{tr} \left[ (\chi^{T_2} \chi)^{T_1} \right] = d^4 \text{tr} \left[ (\chi^{T_2} \chi)^{T_1} \chi^{T_2} \chi \right].
\]
Hence in total if

\[ a_3 = \text{tr} (\chi \chi_0) + 2 \text{tr} \left( \left( \chi \chi_0^T \right)^{\dagger} \left( \chi \chi_0^T \right) \right), \]

\[ b_3 = 2 \text{tr} (\chi^2 \chi_0) + \text{tr} (\chi \chi_0^T) + \text{tr} (\chi^T \chi_0) + 2 \text{tr} (\chi \chi_0) + 2 \text{tr} (\text{tr}_2 [\chi \chi_0 + \chi_0 \chi] \text{tr}_2 [\chi]), \]

\[ c_3 = 4 \text{tr} (\chi \chi_0) + \text{tr} (\chi \chi_0^T) + \text{tr} (\chi^2) + 1 + \text{tr} \left( (\text{tr}_2 \chi)^2 \right), \]

\[ d_3 = 3. \]

then,

\[ \mathcal{F}^2 = \frac{a_3 d^4 + b_3 d^3 + c_3 d^2 + d_3 d}{d^4 + 6d^3 + 11d^2 + 6d}. \] (15)

From Eq. (6) we have,

\[ \mathcal{F}^2 = \frac{a_3 d + b_3 d + 1}{d^2 + 2d + 1}. \] (16)

where,

\[ a = \text{tr} (\chi \chi_0)^2, \]

\[ b = 2 \text{tr} (\chi \chi_0). \]

Taken together, Eq.'s (15) and (16) give the following expression for \( \text{Var} (\mathcal{F}) \),

\[ \text{Var} (\mathcal{F}) = \frac{a_4 d^5 + b_4 d^4 + c_4 d^3 + d_4 d^2 + e_4 d + f_4}{(d + 1)^3(d + 2)(d + 3)} \] (17)

where,
\[ a_4 = a_3 - a, \]
\[ b_4 = b_3 + 2a_3 - b - 6a, \]
\[ c_4 = a_3 + 2b_3 + c_3 - 11a - 6b - 1, \]
\[ d_4 = b_3 + 2c_3 + d_3 - 6a - 11b - 6, \]
\[ e_4 = c_3 + 2d_3 - 11b - 6, \]
\[ f_4 = d_3 - 6. \]

\[ (18) \]

**IV. HIGHER ORDER MOMENTS**

We briefly discuss how to calculate both the higher order moments \( \mathcal{F}^m \) and central moments \( (\mathcal{F} - \mathcal{F})^m \) of the gate fidelity \( \mathcal{F} \). We have already given a detailed analysis of the \( m = 1 \) and \( m = 2 \) cases, and have provided explicit expressions for \( \mathcal{F}^2 \) and \( \text{Var}(\mathcal{F}) = \mathcal{F}^2 - \mathcal{F}^2 \) in terms of the Jamiołkowski state of a quantum operation (note that the first central moment is just \( \mathcal{F} \)). The central moments contain valuable information about the distribution of the gate fidelity. The second central moment (variance) is a measure of the spread of the distribution, the third central moment measures the skewness, and so on. Since the \( m \)'th central moment is just \( (\mathcal{F} - \mathcal{F})^m \) and we have an expression for \( \mathcal{F} \), the expression for the \( m \)'th central moment is easily obtained if each of \( \mathcal{F}^k \) is known for \( k = 1, \ldots, m \).

For \( m \in \mathbb{N} \), the \( m \)'th power of \( \mathcal{F} \), \( \mathcal{F}^m \), has action on pure state \( |\psi\rangle\langle\psi| \),

\[ \mathcal{F}^m (|\psi\rangle\langle\psi|) = \text{tr} (A (|\psi\rangle\langle\psi|) |\psi\rangle\langle\psi|)^m = \sum_{i_1} \text{tr} \left( \left( K_{i_1} \otimes K_{i_1}^\dagger \right) |\psi\rangle\langle\psi| \otimes |\psi\rangle\langle\psi| \right) = \sum_{i_1, \ldots, i_m} \text{tr} \left( \left( K_{i_1} \otimes K_{i_1}^\dagger \otimes \cdots \otimes K_{i_m} \otimes K_{i_m}^\dagger \right) |\psi\rangle\langle\psi| \right). \]

In an analogous method to that used in calculating an expression for the variance, we can use the results regarding permutation operators and the symmetric subspace described in Sec. [II.E] to obtain

\[ \mathcal{F}^m = \frac{1}{\text{tr} (\pi_{\text{sym}} (2m, d))} \sum_{i_1, \ldots, i_m} \text{tr} \left( \left( K_{i_1} \otimes K_{i_1}^\dagger \otimes \cdots \otimes K_{i_m} \otimes K_{i_m}^\dagger \right) \pi_{\text{sym}} (2m, D) \right) = \frac{1}{(2m)! \binom{2m+d-1}{d-1}} \sum_{i_1, \ldots, i_m} \text{tr} (K_{i_1}) \text{tr} (K_{i_1}^\dagger) \cdots \text{tr} (K_{i_m}) \text{tr} (K_{i_m}^\dagger) + \cdots + \text{tr} (K_{i_1} K_{i_1}^\dagger \cdots K_{i_m} K_{i_m}^\dagger). \]
where again the \( \{ K_i \} \) are a set of Kraus operators for \( \Lambda \). There are \( (2^m)! \) terms in the sum corresponding to the fact that there are \( (2^m)! \) elements in the symmetric group \( S_{2m} \) and we have used the fact that,

\[
\text{tr} (\pi_{\text{sym}} (2m, D)) = \binom{2m + d - 1}{d - 1}.
\]

Expanding the \( K_i \) in terms of the basis \( \{ P_i \} \) with the previously discussed properties gives,

\[
\mathcal{F}^m = \frac{1}{(2m)! (\frac{2m + d - 1}{d - 1})} \sum_{i_1, i_2, ..., i_{m_1}, i_{m_2}} \chi_{i_1, i_2} \cdots \chi_{i_{m_1}, i_{m_2}} (\text{tr} (P_{i_1}) \text{tr} (P_{i_2}) \cdots \text{tr} (P_{i_{m_1}}) \text{tr} (P_{i_{m_2}}) + ...)
\]

\[
= \frac{1}{(2m)! (\frac{2m + d - 1}{d - 1})} (\text{tr} (\chi \chi_0)^m d^{2m} + ...).
\]

V. THE SINGLE QUBIT AND LARGE-DIMENSIONAL CASES

In this section we analyze the behavior of \( \text{Var} (\mathcal{F}) \) in two useful cases, that of a single qubit \( (d=2) \) and as \( d \) grows to \( \infty \). The calculations in both cases are straightforward but tedious and so are contained in the appendix. We first look at the case of a single qubit.

For a qubit system, one can obtain much simpler equations for \( \text{Var} (\mathcal{F}) \) than Eq. (17). The calculation involves starting from Eq. (9), grouping certain terms together, and considering various cases. The result of the calculation is that the second moment of \( \mathcal{F} \) is given by,

\[
\mathcal{F}^2 = \frac{-48 \text{tr} (\chi \chi_0)^2 + 64 \text{tr} (\chi \chi_0) + 24 \text{tr} (\chi \chi^T \chi_0 + \chi^T \chi \chi_0) + 32 \text{tr} (\chi^2 \chi_0) + 4 \text{tr} (\chi \chi^T) + 12 \text{tr} (\chi^2) + 4 \text{tr} \left( \left( \text{tr} \chi \right)^2 \right) + 6}{120}.
\]

Using Eq. (16) we obtain the following particularly simple analogue of Eq. (17),

\[
\text{Var} (\mathcal{F}) = -\frac{11}{180} + \frac{4}{45} \text{tr} (\chi \chi_0) - \frac{38}{45} \text{tr} (\chi \chi_0)^2 + \frac{4}{15} \text{tr} (\chi^2 \chi_0) + \frac{1}{10} \text{tr} (\chi^2)
\]

\[
+ \frac{1}{5} \text{tr} (\chi \chi^T \chi_0 + \chi^T \chi \chi_0) + \frac{1}{30} \left( \text{tr} (\chi \chi^T) + \text{tr} \left( \left( \text{tr} \chi \right)^2 \right) \right).
\]

(19)

In the case that \( d \to \infty \), it is relatively straightforward to deduce the behavior of \( \text{Var} (\mathcal{F}) \). The idea is to use a suitable expression for the variance and bound the coefficients of the powers of \( d \). The result is that for large \( d \),
Var (F) \sim \frac{O(d^3)}{O(d^4)} \\
\sim O\left(\frac{1}{d}\right) . \quad (20)

Therefore Var (F) \rightarrow 0 in the inverse of the dimension of the quantum system. A key point here is that Eq. (20) is completely general: for any quantum operation \( E \) and any unitary operation \( U \), the gate fidelity between \( E \) and \( U \) has variance that diminishes as \( O\left(\frac{1}{d}\right) \).

VI. DISCUSSION

We have given a method for calculating all moments of the gate fidelity \( F_{E,U} \) between a unitary \( U \) and a quantum operation \( E \). Using this method we have obtained a closed form, basis-independent, expression for \( \text{Var} (F_{E,U}) \) in terms of the Jamiolkowski state for \( \Lambda = U^\dagger \circ E \). A simple expression for the variance is given in the single qubit case and we have shown that for large quantum systems the variance scales as \( O\left(\frac{1}{d}\right) \) for any \( E \) and \( U \).

There is growing interest in the use of twirling [9, 10] and randomization methods [6, 11] to estimate partial information about the unknown noise affecting the implementation of quantum memory or quantum gates in a completely scalable manner [12, 13]. 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 [11] 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 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 [10] 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 [6], 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 [6] 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 $\chi$-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 raises 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 [14] 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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A. VARIANCE FOR A SINGLE QUBIT

In this section Var(\(\mathcal{F}\)) 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 Eq. (6) we only need to calculate \(\mathcal{F}^2\). We will use Eq. (9) which will allow us to group particular terms together to obtain a more simple expression.

To begin, we recall some properties of \(\chi\). First, \(\chi\) is positive and has trace equal to 1. Second, \(\sum_{l,m} \chi_{l,m} P_l P_m = \Lambda(\mathbb{I}) = d\Lambda\left(\frac{l}{d}\right)\), and third, \(\sum_{l,m} \chi_{l,m} P_m P_l = 1\) from trace preservation. The 24 terms in Eq. (9) 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. Note that many of the expressions below only hold under the assumption that \(d = 2\).

1. First Group of Terms

The first group consists of the following 10 terms:

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

where for ease of presentation we have used square brackets “[ ]” to represent the trace operation. Using the assumed properties of the \(\{P_i\}\) basis this group can be written as,

\[
16 \left( \chi_{0,0}^2 + \sum_l \chi_{0,l} \chi_{l,0} + \chi_{0,0} \right) + 8 \left( \sum_l (\chi_{0,l}^2 + \chi_{l,0}^2) \right) + 4 \left( \sum_{l,m} (\chi_{l,m}^2 + \chi_{l,m} \chi_{m,l}) + 1 \right). \tag{A1}
\]

2. Second Group of Terms

The second group consists of the 8 terms

\[
\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr}(P_l P_r P_n) \text{tr}(P_m) + \text{tr}(P_l P_m P_r) \text{tr}(P_n) + \text{tr}(P_m P_r P_n) \text{tr}(P_l) + \text{tr}(P_m P_n P_r) \text{tr}(P_l)) \\
+ \text{tr}(P_l P_m P_r) \text{tr}(P_n) + \text{tr}(P_l P_m P_n P_r) \text{tr}(P_m) + \text{tr}(P_m P_l P_m) \text{tr}(P_r) + \text{tr}(P_n P_l P_m) \text{tr}(P_r)).
\]

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 $P_nP_r = -P_rP_n$ and so the above is 0.

Case 2: $n = r$. We get $2 \sum_{l,m,n} \chi_{l,m} \chi_{n,n} \text{tr } (P_l) \text{tr } (P_m)$ which equals $2\chi_{0,0}d^2$.

Case 3: $n = 0$. We get, $2 \sum_{l,m,r} \chi_{l,m} \chi_{0,r} \text{tr } (P_lP_r) \text{tr } (P_m)$ which is just $2 \sum_l \chi_{l,0} \chi_{0,l}d^2$.

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

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

Hence the five cases give in total,

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr } (P_lP_rP_nP_m) + \text{tr } (P_lP_nP_rP_m) + \text{tr } (P_lP_nP_mP_r) + \text{tr } (P_lP_rP_mP_n)) + \text{tr } (P_lP_mP_rP_n) + \text{tr } (P_lP_mP_nP_r)$$

which we group into three pairs as,

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr } (P_lP_rP_nP_m) + \text{tr } (P_lP_rP_mP_n))$$

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr } (P_lP_rP_nP_m) + \text{tr } (P_lP_rP_mP_n))$$

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr } (P_lP_rP_nP_m) + \text{tr } (P_lP_rP_mP_n)) + \text{tr } (P_lP_mP_rP_n) + \text{tr } (P_lP_mP_nP_r)$$

The other three sums are calculated in a similar fashion and in total,

$$8\chi_{0,0}d^2 + 8 \sum_l \chi_{l,0} \chi_{0,l}d^2 + 4 \sum_l \chi_{l,0}^2 d^2 + 4 \sum_l \chi_{l,0}^2 d^2 + 16 \chi_{0,0}^2 d^2.$$  

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

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

(A2)

3. Third Group of Terms

Lastly we have the 6 terms

$$\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr } (P_lP_rP_nP_m) + \text{tr } (P_lP_nP_rP_m) + \text{tr } (P_lP_nP_mP_r) + \text{tr } (P_lP_rP_mP_n)) + \text{tr } (P_lP_mP_rP_n) + \text{tr } (P_lP_mP_nP_r))$$

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

and

\[
\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr} (P_l P_m P_n P_r) + \text{tr} (P_l P_n P_m P_r))
\]

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

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

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: \(m = n\). In this case the pair becomes \(4 \sum_{l,m} \chi_{l,m} \chi_{m,l}\).

Case 3: \(m = 0\). The pair becomes \(2 \sum_{l,n,r} \chi_{l,0} \chi_{n,r} \text{tr} (P_l P_n P_r)\) and after a direct calculation,

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

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 \(n = 0\). This case gives \(4 \sum_l \chi_{l,0} \chi_{0,l}\).

Combining the 5 cases gives,

\[
\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr} (P_l P_n P_m P_r) + \text{tr} (P_l P_m P_n P_r)) = 4 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 8 \chi_{0,0}
\]

\[
+ 4 (\chi_{0,1} + \chi_{1,0}) (\chi_{0,1} + \chi_{1,0} + i (\chi_{2,3} - \chi_{3,2})) + 4 (\chi_{0,2} + \chi_{2,0}) (\chi_{0,2} + \chi_{2,0} + i (\chi_{3,1} - \chi_{1,3}))
\]

\[
+ 4 (\chi_{0,3} + \chi_{3,0}) (\chi_{0,3} + \chi_{3,0} + i (\chi_{1,2} - \chi_{2,1})) - 8 \sum_l \chi_{0,l} \chi_{l,0}
\]
The third pair can be expressed as,

$$
\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr} (P_l P_m P_n) + \text{tr} (P_l P_m P_n)) = \text{tr} \left( \Lambda^\dagger (\Lambda^\dagger (\mathbb{1})) \right) + \text{tr} (\Lambda (\Lambda (\mathbb{1}))) = 4
$$

and so combining the three pairs gives,

$$
8 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 16 \chi_{0,0} - 16 \sum_l \chi_{l,0} \chi_{0,l} + 4 + 4 (\chi_{0,1} + \chi_{1,0}) (\chi_{0,1} + \chi_{1,0} + i (\chi_{2,3} - \chi_{3,2}))
$$

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

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

$$
\text{tr} (\Lambda (\Lambda^\dagger (\mathbb{1}))) + \text{tr} (\Lambda^\dagger (\Lambda (\mathbb{1}))) + \text{tr} (\Lambda^\dagger (\Lambda^\dagger (\mathbb{1}))) + \text{tr} (\Lambda (\Lambda (\mathbb{1}))) = 3d + \text{tr} (\Lambda^\dagger (\Lambda (\mathbb{1}))) = 6 + \text{tr} \left( \Lambda (\mathbb{1})^2 \right)
$$

with the remaining two terms, \( \sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} \text{tr} (P_l P_m P_n) \) and \( \sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} \text{tr} (P_l P_m P_n) \), being complex conjugates of one another. From the calculation of the first pair given above,

$$
\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} (\text{tr} (P_l P_m P_n) + \text{tr} (P_l P_m P_n)) = 4 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 8 \chi_{1,1} - 8 \sum_l \chi_{l,1} \chi_{1,l},
$$

and since \( \sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} \text{tr} (P_l P_m P_n) = 2 \),

$$
\sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} \text{tr} (P_l P_m P_n) = \sum_{l,m,n,r} \chi_{l,m} \chi_{n,r} \text{tr} (P_l P_m P_n) = 4 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 8 \chi_{0,0} - 8 \sum_l \chi_{l,0} \chi_{0,l} - 2.
$$

Therefore the three pairs can also be written as

$$
2 + \text{tr} \left( \Lambda (\mathbb{1})^2 \right) + 8 \sum_{l,m} \chi_{l,m} \chi_{m,l} + 16 \chi_{0,0} - 16 \sum_l \chi_{l,0} \chi_{0,l}, \quad \text{(A3)}
$$

where by Eq. (11),

$$
\text{tr} \left( \Lambda (\mathbb{1})^2 \right) = 4 \text{tr} ((\text{tr} 2 \chi )^2) = 2 + 4 (\chi_{0,1} + \chi_{1,0}) (\chi_{0,1} + \chi_{1,0} + i (\chi_{2,3} - \chi_{3,2}))
$$

$$
+ 4 (\chi_{0,2} + \chi_{2,0}) (\chi_{0,2} + \chi_{2,0} + i (\chi_{3,1} - \chi_{1,3})) + 4 (\chi_{0,3} + \chi_{3,0}) (\chi_{0,3} + \chi_{3,0} + i (\chi_{1,2} - \chi_{2,1})).
$$
Combining all 24 terms given in Eq.’s (A1), (A2) and (A3), and noting \( \text{tr}(\pi_{\text{sym}}(4,d)) = \frac{120}{24} \),

\[
F^2 = \left( -48\chi^2_{0,0} + 64\chi_{0,0} + 24(\chi\chi^T + \chi^T\chi)_{0,0} + 32(\chi^2)_{0,0} + 4\text{tr}(\chi\chi^T) + 12\text{tr}(\chi^2) + 6 + 4\text{tr}((\text{tr}\chi)^2) \right) \frac{120}{24}.
\] (A4)

**B. VARIANCE IN LARGE DIMENSIONS**

To deduce the asymptotic behavior of \( \text{Var}(F) \) we use the expression for \( F^2 \) given in Eq. (10). From this equation one can obtain the following expression for \( \text{Var}(F) \),

\[
\text{Var}(F) = \frac{rd^4 + sd^3 + ud^2 + vd + w}{d(d^2 + 2d + 1)(d^2 + 5d + 1)}.
\] (B1)

where,

\[
\begin{align*}
 r &= -4\chi^2_{0,0} + (\chi\chi^T)_{0,0} + (\chi^T\chi)_{0,0} + 2(\chi^2)_{0,0}, \\
 s &= -6\chi^2_{0,0} + (\chi\chi^T)_{0,0} + (\chi^T\chi)_{0,0} + \text{tr}(\chi\chi^T) - 4\chi_{0,0} + \text{tr}(\chi^2) + 2(\chi^2)_{0,0}, \\
 u &= -8\chi_{0,0} + \text{tr}(\chi\chi^T) + \text{tr}(\chi^2) + 2\text{tr}\left(\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \Lambda(\mathbb{I})\right) - 1, \\
 v &= 2\text{tr}\left(\sum_{l,m} \chi_{l,m} P_l \Lambda(\mathbb{I}) \right) + 2\text{tr}\left(\sum_l (\chi_{l,0} + \chi_{0,l}) P_l \Lambda(\mathbb{I})\right) + \text{tr}\left((\Lambda(\mathbb{I}))^2\right) - 3, \\
 w &= 2\text{tr}\left(\sum_{l,m} \chi_{l,m} P_l \Lambda(\mathbb{I}) \right) + \text{tr}\left((\Lambda(\mathbb{I}))^2\right).
\end{align*}
\]

The denominator of (B1) is a quintic polynomial in \( d \). The numerator contains powers of \( d \) up to and including \( d^4 \), however the coefficients depend on \( \chi \). We would like to bound these coefficients in terms of \( d \).

First, since \( \chi \) is a trace-1 positive semi-definite matrix, we obtain the bounds \( 0 \leq \chi^2_{0,0} \leq \chi_{0,0} \leq 1 \) and \( 0 \leq \text{tr}(\chi^2) \leq \text{tr}(\chi) = 1 \). Next, for a linear operator \( A \), the Frobenius (Hilbert-Schmidt) norm of \( A \), denoted by \( ||A||_F \), is given by \( ||A||_F = \sqrt{\text{tr}(A^\dagger A)} \). Using the Cauchy-Schwarz inequality we obtain,

\[
\left|\text{tr}(\chi\chi^T)\right| \leq ||\chi||_F ||\chi^T||_F.
\]
Since $\chi$ and $\chi^T$ have the same singular values, $\|\chi\|_F = \|\chi^T\|_F$. Therefore $\|\chi\|_F \leq 1 \Rightarrow |\text{tr} (\chi \chi^T)| \leq 1$. This also implies $|\langle \chi \chi^T \rangle_{0,0}| \leq 1$ and $|\langle \chi^T \chi \rangle_{0,0}| \leq 1$. To deal with $\Lambda (I)$, we note that it has trace $d$ and is positive semi-definite. Hence $0 \leq \text{tr} \left( (\Lambda (I))^2 \right) \leq d^2$.

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

$$\left| \text{tr} \left( \sum_l \chi_{l,0} P_l \Lambda (I) \right) \right| \leq \left\| \sum_l \chi_{l,0} P_l \right\|_F \left\| \Lambda (I) \right\|_F \leq d \left\| \sum_l \chi_{l,0} P_l \right\|_F.$$

Since,

$$\left\| \sum_l \chi_{l,0} P_l \right\|_F = \sqrt{\text{tr} \left( \left( \sum_l \chi_{l,0} P_l \right)^\dagger \left( \sum_m \chi_{m,0} P_m \right) \right)} = \sqrt{\text{tr} \left( \left( \sum_l \chi_{l,0} P_l \right) \left( \sum_m \chi_{m,0} P_m \right) \right)}$$

$$= d \langle \chi^2 \rangle_{0,0} \leq d$$

we get $|\text{tr} \left( \sum_l (\chi_{l,0} + \chi_{0,l}) P_l \Lambda (I) \right)| \leq 2d^2$.

Finally, we need to bound $\text{tr} \left( \sum_{l,m} \chi_{l,m} P_l \Lambda (P_m) \right)$. Using Eq. [13] we have $\text{tr} \left( \sum_{l,m} \chi_{l,m} P_l \Lambda (P_m) \right) = d^2 \text{tr} \left( S (S \chi)^T_1 \chi \right)$ where $S$ is the unitary Kraus operator for the SWAP gate. Again, by the Cauchy-Schwarz inequality,

$$\left| \text{tr} \left( \chi S (S \chi)^T_1 \right) \right| \leq \|\chi S\|_F \left\| (S \chi)^T_1 \right\|_F = \sqrt{\text{tr} \left( (\chi S) (\chi S)^\dagger \right)} \sqrt{\text{tr} \left( ((S \chi)^T_1)^\dagger (S \chi)^T_1 \right)}$$

$$\leq \sqrt{\text{tr} \left( ((S \chi)^T_1)^\dagger (S \chi)^T_1 \right)}$$

since $\sqrt{\text{tr} \left( (\chi S) (\chi S)^\dagger \right)} = \sqrt{\text{tr}(\chi^2)} = \|\chi\|_F \leq 1$. For any $A, B \in L(\mathcal{H} \otimes \mathcal{H})$, $(A^\dagger)^T_1 = (A^T_1)^\dagger$ and $\text{tr} \left( (AB)^T_1 \right) = \text{tr} \left( (B^T_1 A^T_1) \right)$. Therefore,

$$\text{tr} \left( ((S \chi)^T_1)^\dagger (S \chi)^T_1 \right) = \text{tr} \left( (S \chi)^T_1 (S \chi)^T_1 \right) = \text{tr} \left( (S \chi)^T_1 (S \chi)^T_1 \right)$$

$$= \text{tr} \left( (S \chi)^T_1 (S \chi)^T_1 \right) = \text{tr} (\chi^2) \leq 1,$$

which implies $|\text{tr} \left( \sum_{l,m} \chi_{l,m} P_l \Lambda (P_m) \right)| \leq d^2$. 


Combining all of these results implies that the numerator of \( B1 \) is quartic in \( d \) and so for large \( d \),

\[
\text{Var}(F) \sim \frac{O(d^3)}{O(d^3)} = O\left(\frac{1}{d}\right) .
\] (B2)
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