The Accuracy vs. Sampling Overhead Trade-off in Quantum Error Mitigation Using Monte Carlo-Based Channel Inversion

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Abstract—Quantum error mitigation (QEM) is a class of promising techniques for reducing the computational error of variational quantum algorithms. In general, the computational error reduction comes at the cost of a sampling overhead due to the variance-boosting effect caused by the channel inversion operation, which ultimately limits the applicability of QEM. Existing sampling overhead analysis of QEM typically assumes exact channel inversion, which is unrealistic in practical scenarios. In this treatise, we consider a practical channel inversion strategy based on Monte Carlo sampling, which introduces additional computational error that in turn may be eliminated at the cost of an extra sampling overhead. In particular, we show that when the computational error is small compared to the dynamic range of the error-free results, it scales with the square root of the number of gates. By contrast, the error exhibits a linear scaling of the error-free results, it scales with the square root of the number of gates. By contrast, the error exhibits a linear scaling of the error-free results, it scales with the square root of the number of gates. In particular, we show that when this treatise, we consider a practical channel inversion strategy based on Monte Carlo sampling, which introduces additional computational error that in turn may be eliminated at the cost of an extra sampling overhead. In particular, we show that when this treatise, we consider a practical channel inversion strategy based on Monte Carlo sampling, which introduces additional computational error that in turn may be eliminated at the cost of an extra sampling overhead. In particular, we show that when this treatise, we consider a practical channel inversion strategy based on Monte Carlo sampling, which introduces additional computational error that in turn may be eliminated at the cost of an extra sampling overhead. In particular, we show that when this treatise, we consider a practical channel inversion strategy based on Monte Carlo sampling, which introduces additional computational error that in turn may be eliminated at the cost of an extra sampling overhead. In particular, we show that when this treatise, we consider a practical channel inversion strategy based on Monte Carlo sampling, which introduces additional computational error that in turn may be eliminated at the cost of an extra sampling overhead.

ACRONYMS

- MSE: Mean-Square Error
- PTM: Pauli Transfer Matrix
- QEM: Quantum Error Mitigation
- RMSE: Root-Mean-Square Error
- VQA: Variational Quantum Algorithm

NOTATIONS

- Deterministic scalars, vectors and matrices are represented by \( x \), \( \mathbf{x} \), and \( \mathbf{X} \), respectively, whereas their random counterparts are denoted as \( x \), \( \mathbf{x} \), and \( \mathbf{X} \), respectively. Deterministic sets, random sets, and operators are denoted as \( \mathcal{X} \), \( \mathbf{X} \), and \( \mathcal{X} \), respectively.
- The notations \( 1_n, 0_n, 0_{m \times n}, \text{ and } I_k \), represent the \( n \)-dimensional all-one vector, the \( n \)-dimensional all-zero vector, the \( m \times n \) dimensional all-zero matrix, and the \( k \times k \) identity matrix, respectively. The subscripts may be omitted if they are clear from the context.
- The notation \( \| x \|_p \) represents the \( \ell_p \)-norm of vector \( x \), and the subscript may be omitted when \( p = 2 \). For matrices, \( \| A \|_p \) denotes the matrix norm induced by the corresponding \( \ell_p \) vector norm. The notation \( 1/x \) represents the element-wise reciprocal of vector \( x \).
- The notation \( [A]_{i,j} \) denotes the \((i,j)\)-th entry of matrix \( A \). For a vector \( x \), \([x]_i\) denotes its \( i \)-th element. The submatrix obtained by extracting the \( i_1 \)-th to \( i_2 \)-th rows and the \( j_1 \)-th to \( j_2 \)-th columns from \( A \) is denoted as \([A]_{i_1:i_2,j_1:j_2}\). The notation \([A]_{:,i}\) represents the \( i \)-th column of \( A \), and \([A]_{i,:}\) denotes the \( i \)-th row, respectively.
- The trace of matrix \( A \) is denoted as \( \text{Tr}(A) \), and the complex conjugate of \( A \) is denoted as \( A^\dagger \). Similarly, the complex adjoint of an operator \( \mathcal{X} \) is also denoted as \( \mathcal{X}^\dagger \).
- The notation \( A \otimes B \) represents the Kronecker product between matrices \( A \) and \( B \). The notation \( A \circ B \) denotes the Hadamard product between matrices \( A \) and \( B \).
- The notations \( E\{\cdot\} \), \( \text{Var}\{\cdot\} \), and \( \text{Cov}\{\cdot\} \) represent the expectation, the variance, and the covariance matrix of their arguments, respectively.

I. INTRODUCTION

NOisy intermediate-scale quantum computers [1] has been one of the most impressive recent advances in the area of quantum computing. In particular, a quantum computer consisting of 53 quantum bits (qubits) has been built in 2019, and has been shown being capable of performing computational tasks that are challenging to be carried out by state-of-the-art classical supercomputers [2]. Due to their limited number of qubits, noisy intermediate-scale quantum computers may not be capable of supporting fully fault-tolerant quantum operations relying on quantum error correction codes [3]–[6], which are widely believed to be necessary for implementing complex algorithms that require relatively long coherence time [7]–[9], such as Shor’s factorization algorithm [10] and Grover’s search algorithm [11]. Alternatively, a class of algorithms tailored for these computers, namely that of the variational quantum algorithms (VQAs) [12]–[15], is receiving much attention. Briefly, VQAs aim for sharing their computational tasks between relatively simple quantum circuits and classical computers. A little more specifically, quantum circuits are employed in VQA for computing a cost function or its gradient [16], which is then fed into an optimization algorithm run on classical computers. The objective of this design paradigm is to assist near-term quantum devices in outperforming classical computers in the context of practical problems, such as solving combinatorial optimization problems using the quantum approximate optimization algorithm [14], [17], [18] and quantum chemistry problems using the variational quantum eigensolver [12]. Although the performance of VQAs has been characterized using some illustrative examples [12], [24]–[26], it is not known whether these examples could be scaled up to problems of larger size. In fact, recent analytical results in [19], [27], [28] support the opposite statement. More explicitly, [19]...
proves that the magnitude of the cost function (or its gradient) computed by VQAs vanishes exponentially as the number of qubits $n$ increases. Fortunately, the follow-up investigations [29], [30] found that this so-called “barren plateau” phenomenon may be mitigated to a certain extent by techniques borrowed from the literature of classical machine learning, such as pre-training and layer-by-layer training. However, the authors of [20] show that when decoherence is taken into account, the dynamic range of the computational results also vanishes exponentially upon increasing the circuit depth $N_l$, even if these techniques are applied. To summarize, these results imply that when the quantum circuit is long in depth or large in the number of qubits, the computational error become excessive in practical applications.

To improve the error scaling of VQAs with respect to the depth of the circuits, a body of literature has been devoted to searching for methods that efficiently mitigate the effect of decoherence-induced impairment, without using quantum error correction codes [31]–[34]. Among these research efforts, one of the most promising methods is quantum error mitigation (QEM) [31], which aims for applying an “inverse channel” right after each quantum channel modelling the impact of decoherence. Both the numerical and experimental results of [21], [35] show that QEM is indeed capable of reducing the computational error in VQAs in the context of quantum chemistry problems.

The error reduction capability of QEM comes at the price of a computational overhead. To elaborate, QEM is implemented by sampling from a “quasi-probability representation” of the inverse channel, which would increase the variance of the computational results, hence some computational overhead (termed as “sampling overhead” [21], [22]) is required for ensuring that a satisfactory accuracy can be achieved. By appropriately choosing the total number of samples, one may strike a beneficial computational accuracy vs. overhead trade-off. Therefore, it is important to quantify the sampling overhead, before we can conclude whether QEM can play a significant role in making VQAs practical.

The literature of QEM sampling overhead analysis typically assumes that the channel inversion procedure is implemented exactly [21]–[23] Under this assumption, the sampling overhead can be characterized by the sampling overhead factor $\epsilon_n$, which is determined by the quality of the channel as well as with the gate error probability $\epsilon$. We boldly and explicitly contrast our contributions to the related recent research on VQAs and QEM in Table I which are further detailed as follows.

- We analyse the error scaling in the absence of QEM, by providing both upper and lower bounds of the magnitude of the computational error. We show that the error magnitude scales linearly with the number of gates $N_G$, as well as with the gate error probability $\epsilon$, when we have $\epsilon N_G \ll 1$.
- We propose an upper bound on the root-mean-square error (RMSE) of the computational error in the presence of Monte Carlo-based QEM. Specifically, we show that the RMSE is upper bounded by the square root of $N_G$, as well as $\epsilon$, when $\epsilon N_G \ll 1$. This implies that when we use the same number of samples as the ideal QEM, Monte Carlo-based QEM can still provide a quadratic error reduction versus $N_G$, compared to the case of no QEM.
- We provide an intuitive interpretation of the proposed error scaling laws, by visualizing the decoherence-induced impairments on the Bloch sphere as the quantum circuit executes.
- We demonstrate the analytical results using various numerical examples. Specifically, we consider a practical

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TABLE I

| Circuit condition | Subject of Analysis | Method of performance evaluation |
|-------------------|---------------------|----------------------------------|
| Noisy? | QEM implementation | Only accuracy | Only numerical |
| J. R. McClean et al. | × | No QEM | Analytical and numerical |
| J. R. McClean et al. | × | No QEM | Analytical and numerical |
| S. Wang et al. | ✓ | No QEM | Analytical and numerical |
| S. Endo et al. | ✓ | Exact channel inversion | Only numerical |
| Y. Xiong et al. | ✓ | Exact channel inversion | Analytical and numerical |
| R. Takagi | ✓ | Exact channel inversion | Analytical and numerical |
| Our contributions | ✓ | Monte Carlo-based channel inversion | Analytical and numerical |

1 We will refer to QEM based on exact channel inversion as “ideal QEM” in the rest of this treatise.
application of carrying out multiuser detection in wireless communication systems using the quantum approximate optimization algorithm and show that our analytical results do apply.

The rest of this treatise is organized as follows. In Section II, we present the formulation of VQAs and the channels modelling the decoherence. Then, in Section III we discuss a pair of QEM implementation strategies, namely the Monte Carlo-based QEM and the exact channel inversion. Based on this discussion, in Section IV we analyse the error scaling behaviours of these two QEM implementations, respectively, under the assumption that they use the same number of circuit executions. We provide further intuitions concerning these analytical results in Section V with an emphasis on the accuracy vs. sampling overhead trade-off, complemented by numerical examples in Section VI. Finally, we conclude in Section VII.

II. FORMULATION OF VARIATIONAL QUANTUM ALGORITHMS

A typical VQA iterates between classical and quantum devices, as portrayed in Fig. 1. The parametric state-preparation circuit (also known as the “ansatz”) transforms a fixed input state to an output state, according to the parameters chosen by a classical optimizer. The output state is then measured and fed into a quantum observable, which maps the measurement outcomes to the desired computational results. The results correspond to the value of a cost function or its gradient, which in turn serve as the input of the associated classical optimization algorithm. The iterations continue until certain stopping criterion is met, for example, the computed gradient becomes almost zero.

In this treatise, we focus on the error induced by the sampling procedure in QEM, hence we consider the computational result of a single iteration, meaning that the parameters used for state preparation are fixed. We model the decoherence-induced impairment in the parametric state-preparation circuit as quantum channels acting upon the associated quantum states at the output of perfect quantum gates, as exemplified by the simple circuit shown in Fig. 2. In this figure, \( C_k \), \( k = 1 \ldots 4 \) represents the channel modelling the decoherence in the \( k \)-th quantum gate, while \( G_k \) represents the \( k \)-th ideal decoherence-free quantum gate.

In the subsequent subsections, we present the mathematical formulations of the system models shown in Fig. 1 and 2.

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![Diagram](image-url)  
**Fig. 1.** The structure of a typical implementation for variational quantum algorithms.

![Diagram](image-url)  
**Fig. 2.** Simple example of the noisy parametric state-preparation circuit seen in Fig. 1.

### A. Operator-sum Representation

Without loss of generality, we assume that the input state of the circuit is the all-zero state \( |0\rangle^\otimes n \), where \( n \) is the number of qubits. In general, when the circuit is decoherence-free, the computational result of a variational quantum circuit may be expressed as

\[
\tilde{\rho} = (|0\rangle\langle 0|)^\otimes n \sum_{E}^N \mathcal{M}_{ob} \prod_{k=1}^{N_G} G_k \prod_{k=1}^{N_G} G_k \prod_{k=1}^{N_G} |0\rangle\langle 0| \,,
\]

where \( N_G \) is the number of gates in the circuit, \( G_k \) denotes the \( k \)-th quantum gate, and the operator \( \mathcal{M}_{ob} \) represents the quantum observable, which describes the computational task as a linear function of the final state.

If we consider a more practical scenario, where the quantum state evolves owing to quantum decoherence as the circuit operates, the state can no longer be fully characterized using the state vector formalism. Instead, we may use the density matrix formalism. In particular, the input state may be described as

\[
\rho_0 = (|0\rangle\langle 0|)^\otimes n \,.
\]

Correspondingly, the output state of the \( k \)-th imperfect quantum gate may be represented in an operator-sum form [36 Sec. 8.2.4], relying on following recursive relationship

\[
\rho_k = C_k \left( G_k \rho_{k-1} G_k^\dagger \right) \,,
\]

where the operator \( C_k \) is characterized by

\[
C_k (\rho) = \sum_{i=1}^{n_k} \left( E_{k,i} \rho E_{k,i}^\dagger \right) \,,
\]

representing the channel modelling the imperfection of the \( k \)-th gate. The matrices \( E_{k,i} \) represent the operation elements [36 Sec. 8.2.4] of the channel \( C_k \) satisfying the completeness condition of \( \sum_{i=1}^{n_k} E_{k,i} E_{k,i}^\dagger = I \). Finally, when all gates
completed their tasks and the measurement results have been obtained, the computational result may be expressed as

$$r = \text{Tr} \{ \mathcal{M}_{ob} \rho_{N_G} \}.$$  (5)

### B. Pauli Transfer Matrix Representation

In the standard operator-sum form [36, Sec. 8.2.4], the quantum states are represented by matrices. However, in many applications, such as the error analysis considered in this treatise, it would be more convenient to treat them as vectors. Correspondingly, the quantum channels and gates would then be represented by matrices. To this end, the Pauli transfer matrix (PTM) representation of quantum operators was proposed in [37], which allows a quantum operator $O$ to be expressed as

$$[O]_{i,j} = \frac{1}{2^n} \text{Tr} \{ S_i O S_j \},$$  (6)

where $S_i$ denotes the $i$-th Pauli operator in the $n$-qubit Pauli group. Similarly, a quantum state $\rho$ can be expressed as

$$[\rho]_i = \frac{1}{\sqrt{2^n}} \text{Tr} \{ S_i \rho \}. $$  (7)

Under the PTM representation, the computational result may be rewritten as

$$r = v_{ob}^T \left( \prod_{k=1}^{N_G} (C_{N_G-k+1} G_{N_G-k+1}) \right) v_0,$$  (8)

where $G_k$ represents the $k$-th perfect gate, and $C_k$ represents the channel modelling the imperfection of the $k$-th gate. The vector $v_0$ denotes the initial state, whereas $v_{ob}$ is the vector representation of the quantum observable $\mathcal{M}_{ob}$.

To simplify the notation, we define

$$R_k := \prod_{i=1}^{k} (C_{k-i+1} G_{k-i+1}),$$  (9)

$$\tilde{R}_k := \prod_{i=1}^{k} G_{k-i+1}.$$  (9)

Especially, for $k = 0$, we define $R_0 = \tilde{R}_0 = I$. The output state of the $k$-th quantum gate can then be expressed as

$$v_k := R_k v_0 = C_k G_k v_{k-1}. $$  (10)

Hence we have

$$r = v_{ob}^T v_{NG} = v_{ob}^T R_{NG} v_0.$$  (11)

### C. Channel Model

In this treatise, we consider Pauli channels [38], for which the Pauli transfer matrices take the following form

$$C_k = \text{diag} \{ c_k \},$$  (12)

where

$$c_k = \tilde{H} p_k,$$  (13)

with $\tilde{H}$ denoting the Hadamard transform, whereas $p_k$ represents a probability distribution satisfying $1^T p_k = 1$, $p_k \geq 0$.

### III. QEM and Its Implementation Strategies

Ideally, for a channel $C_k$, QEM would apply its inverse based on a linear combination of predefined quantum operations, taking the following form

$$C_k^{-1} = \sum_{l=1}^{L} c_l^{(k)} O_l,$$  (14)

where $O_l$ is the $l$-th quantum operation, while $\alpha_k := [\alpha_1 \ldots \alpha_L]^T$ is the quasi-probability representation vector satisfying $1^T \alpha_k = 1$. This linear combination may be rewritten as a probabilistic mixture of the quantum operations as follows:

$$C_k^{-1} = ||\alpha_k||_1 \sum_{l=1}^{L} s_l^{(k)} p_l^{(k)} O_l,$$  (15)

where $s_l^{(k)}$ and $p_l^{(k)}$ are the $l$-th entries of $s_k$ and $p_k$, respectively, given by

$$p_l^{(k)} = \frac{|c_l^{(k)}|}{||\alpha_k||_1},$$  (16)

$$s_k = \text{sgn}(\alpha_k).$$

Note that the vector $p_k$ describes a probability distribution.

Typically, the probabilistic mixture in (15) is implemented by generating a set of candidate circuits and performing post-processing on the output of these circuits. In the following subsections, we will discuss different candidate selection strategies and their characteristics.

#### A. Exact Implementation and Sampling Overhead

The inverse channel $C_k^{-1}$ in (15) is assumed to be implemented exactly in the seminal paper [31] that proposed QEM for the first time, as well as in many other existing contributions [21]–[23]. Exact implementation implies that, each quantum operation $O_l$ should appear in exactly $Np_l^{(k)}$ candidate circuits in every $N$ samples of the computational result.

The assumption of exact implementation significantly simplifies the performance analysis of QEM. In particular, it leads to a clear and concise formula of sampling overhead, which describes the computational overhead imposed by the variance-boosting effect of QEM. To elaborate, assume that the variance of the computational result is $\sigma^2$ based on $N_0$ samples. According to (15), if we implement the inverse channel $C_k^{-1}$, the variance would become $||\alpha_k||_1^2 \sigma^2$. Therefore, in order to achieve the same accuracy as the case without QEM, we should acquire $N_0 (||\alpha_k||_1^2 - 1)$ additional samples. If we further assume that all gates are protected by QEM, we have the following formula for the total sampling overhead

$$N_{\text{exact}} = N_0 \prod_{k=1}^{N_G} \left( ||\alpha_k||_1^2 - 1 \right).$$  (17)

The simplicity of (17) is largely due to the assumption of exact implementation.

Despite its theoretical convenience, the practicality of exact implementation is doubtful. Specifically, the number of the $l$-th candidate circuit, $Np_l^{(k)}$ has to be an integer, which might...
be unrealistic for an arbitrary $p_i^{(K)}$. Furthermore, the number of the probability parameters $p_i^{(K)}$ would increase exponentially as the number of QEM-protected gates increases, which may render the candidate circuit selection procedure computationally prohibitive when $N_G$ is large. Motivated by these drawbacks, we propose to use a Monte Carlo implementation of QEM, detailed in the next subsection.

**B. Monte Carlo Implementation**

In the Monte Carlo implementation, we first sample from the probability distribution $p_i$ for each gate, and obtain $N$ samples constituting a set $L = \{l_1, \ldots, l_N\}$, where for all $k$ we have $l_k = 1, 2, \ldots, L$. Thus we may approximate the inverse channel as

$$r_k = \frac{1}{N} \sum_{i=1}^{N} s_i^{(k)} O_i$$

and

$$= \frac{1}{N} \sum_{i=1}^{L} s_i^{(k)} p_i^{(k)} O_i,$$

where

$$p_i^{(k)} = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}\{l_i = m\}.$$

The advantage of the Monte Carlo approach is that it may result in a much lower complexity for candidate circuit generation, compared to the exact implementation. To elaborate further, as a “toy” example, for a circuit consisting of two gates we have

$$r_2 \tilde{G}_2 \tilde{G}_1 \tilde{G}_1 = \frac{\|\alpha_1\|_1 \|\alpha_2\|_1}{N} \sum_{i=1}^{N} s_i^{(1)} s_i^{(2)} O_i \tilde{G}_2 O_i \tilde{G}_1,$$

where $\tilde{G}_k = C_k G_k$, and $l_{i,k}$ denotes the $i$-th sample drawn from the distribution $p_k$. This implies that in order to obtain a sample for the entire circuit, we may simply generate one sample for each gate, and concatenate them as shown in the right hand side of (19). Compared to the exact implementation, the Monte Carlo implementation can generate an arbitrary number of circuit samples $N$, at a relatively low computational cost of $O(NN_G)$.

The reduced complexity of the Monte Carlo implementation comes with a cost of inaccurate channel inversion, since $G_k$ is only an approximation of $C_k^{-1}$. Hence there would be a residual channel for each gate, which is given by

$$\tilde{C}_k = r_k C_k.$$

A natural question that arises is, whether the additional computational error caused by these residual channels would erode the error reduction capability of Monte Carlo-based QEM. In the rest of this treatise, we will discuss the impact of these residual channels on the accuracy vs. sampling overhead trade-off.

**IV. ERROR SCALING ANALYSIS OF MONTE CARLO-BASED QEM**

In this section, we discuss the error scaling behaviour of quantum circuits protected by Monte Carlo-based QEM, and contrast the results to that of circuits without QEM protection. In order to make a fair comparison, we consider the following assumptions.

**A. Assumptions**

**Assumption 1 (Bounded gate error rate):** The error probability of each quantum gate is upper bounded by $\epsilon$. Since we consider Pauli channels in this treatise, the gate error probability corresponding to a quantum channel $C_k$ (under its PTM representation) may be computed as

$$\epsilon(C_k) = 1 - \frac{1}{4^{n}} \text{Tr} \{C_k\}. \tag{21}$$

**Assumption 2 (Bounded observable):** The eigenvalues of the quantum observable $\mathcal{M}_{ob}$ are bounded in the interval $[-1, 1]$. Assumption 2 ensures the boundedness of the computation result $r$. In this treatise we assume that the upper and lower bounds are 1 and $-1$, respectively, but they may be replaced with any other constant real numbers without affecting our analytical results. The assumption may also be rewritten as

$$\max_{\omega \in S^n} v_{ob}^T \omega v_{ob}^T v_{ob} \leq 1,$$ \tag{22}

where $S^n$ denotes the space of all density matrices over $n$ qubits. Furthermore, the assumption also implies that

$$\|v_{ob}\|_2 \leq \sqrt{2^n}.$$ \tag{23}

This follows from the fact that $\|v_{ob}\|_2 = \|\mathcal{M}_{ob}\|_F$, and that

$$\|\mathcal{M}_{ob}\|_F = \sum_{i=1}^{2^n} \lambda_i(\mathcal{M}_{ob}) \leq \sqrt{2^n},$$

where $\lambda_i(\cdot)$ denotes the $i$-th largest eigenvalue of its argument. **Assumption 3 (Zero bias term):** We assume that

$$\text{Tr} \{\mathcal{M}_{ob}\} = \sqrt{2^n} [v_{ob}]_1 = 0.$$ \tag{24}

Note that $[v_{ob}]_1$ is the coefficient of the identity operator, which serves as a bias term in the computation result being constant with respect to the quantum state. Thus this assumption does not restrict the generality of our results.

**B. Benchmark: Error Scaling in the Absence of QEM**

In this subsections, we characterize the error scaling of quantum circuits that are not protected by QEM. The results will serve as important benchmarks in the following discussions. Let us start with a bound of the dynamic range of computational results, which will lead to a lower bound of the computational error.

**Proposition 1:** Assume that each qubit would be processed by at least $N_l$ gates, and that for each of these gates, the probability of each type of Pauli error (i.e., X error, Y error or Z error) on each qubit is lower bounded by $\epsilon_l$. The computational result $r$ exhibits the following convergence behaviour:

$$|r| \leq \exp(-4\epsilon_l N_l). \tag{25}$$

**Proof:** Please refer to Appendix I. \qed
Proposition 1 implies that decoherence would force the computation result to be almost independent of the quantum observable \( v_{ob} \) in an asymptotic sense. Indeed, as indicated by (23), when \( N_L \) is large, \( r \) is only determined by the first entry of \( v_{ob} \). Moreover, consider the case where \( |\tilde{r}| \geq 1 - c \) holds for all \( N_G \), the computational error is lower bounded as

\[
|r - \tilde{r}| \geq 1 - c - \exp(-4\epsilon_1 N_L).
\]

(26)

From the Taylor expansion

\[
\exp(-4\epsilon_1 N_L) = 1 - 4\epsilon_1 N_L + \frac{(4\epsilon_1 N_L)^2}{2} - \cdots,
\]

we see that when \( \epsilon_1 N_L \ll 1 \), the lower bound is approximately

\[
|r - \tilde{r}| \gtrapprox 4\epsilon_1 N_L - c,
\]

(27)

which increases linearly with respect to \( \epsilon_1 N_L \).

We may also provide an upper bound for the computational error as follows.

**Proposition 2:** The computational error can be upper bounded as

\[
|r - \tilde{r}| \leq 2\epsilon_u N_G.
\]

(28)

**Proof:** Please refer to Appendix II.

\[
\square
\]

Combining Propositions 1 and 2 we see that the computational error grows linearly with \( N_G \), when the number of gates in each “layer” is constant (hence \( N_L \) is a constant multiple of \( N_G \)). This is typically true for VQAs.

### C. The Statistics of the Residual Channels

Before diving into details about the error scaling, in this subsection, we first investigate the characteristics of the residual channels of gates protected by Monte Carlo-based QEM.

According to the sampling overhead analysis in [22] based on the assumption of exact channel inversion, if we wish to execute the decoherence-free circuit \( N \) times, we should sample from the probabilistic mixture of candidate circuits for as many as

\[
N = N_L \|\alpha_k\|^2_1
\]

(29)
times, in order to keep the variance of the computational result unchanged by the channel inversion procedure. Here we consider the Monte Carlo-based channel inversion using the same number of samples, hence we have

\[
\tilde{p}^{(k)}_m = \frac{1}{N_s \|\alpha_k\|^2_1} \sum_{i=1}^{N_s} \Gamma_{m,i}. \quad (30)
\]

Of course, the Monte Carlo-based channel inversion has lower accuracy compared to the exact channel inversion, when they use the same number of samples. The accuracy could be improved by using additional samples, which will be discussed in more detail in Section V.B.

After the sampling procedure, \( \alpha_k \) is approximated by \( \bar{\alpha}_k \) taking the following form

\[
\bar{\alpha}_k = \|\alpha_k\|^2_1 \cdot s_k \odot \tilde{p}_k = \|\alpha_k\|^2_1 \cdot s_k \odot (p_k + n) = \alpha_k + \|\alpha_k\|^2_1 \cdot s_k \odot n,
\]

(31)

where \( n \) denotes the sampling error. In general, the approximated inverse channel may be expressed in terms of \( \bar{\alpha}_k \) as

\[
\Gamma_k = \sum_{i=1}^{L} [\alpha_k]_i O_i,
\]

(32)

where \( \{O_i\}_{i=1}^{L} \) is a set of operators forming a basis of the space where the imperfect gate \( C_k G_k \) resides in. Interested readers may refer to Table 1 in [22] for an example of such operator sets. For the Pauli channels considered in this treatise, \( \Gamma \) has a simpler form. Specifically, using (12), the quasi-probability representation vector may be expressed as

\[
\alpha_k = \tilde{H}^{-1}(1/c_k),
\]

where \( \tilde{H} \) is the Hadamard transform over \( n \) qubits, and \( \tilde{H}^{-1} \) is the corresponding inverse transform given by \( \tilde{H}^{-1} = \frac{1}{N} \tilde{H}^T \).

The approximated inverse channel can now be expressed as

\[
\Gamma_k = \text{diag}^{-1}\{\tilde{H} \bar{\alpha}_k\},
\]

(33)

and thus the residual channel takes the following form

\[
\bar{c}_k = \text{diag}^{-1}\{\tilde{H} \bar{\alpha}_k \odot c_k\}.
\]

(34)

To simplify our further analysis, we introduce \( \bar{c}_k := \tilde{H} \bar{\alpha}_k \odot c_k \), where \( \bar{c}_k \) may be further expressed as

\[
\bar{c}_k = 1 + \|\alpha_k\|^2_1 \cdot \tilde{H} (s_k \odot n) \odot c_k = 1 + \|\alpha_k\|^2_1 \cdot c_k \odot \bar{n},
\]

(35)

and \( \bar{n} := \tilde{H} (s_k \odot n) \). Note that the vector \( \bar{p}_k \) is a multinomial distributed random vector, satisfying

\[
\mathbb{E}\{\bar{p}_k\} = p_k, \quad \text{Cov}\{\bar{p}_k\} = \frac{1}{N_s \|\alpha_k\|^2_1} (P_k - p_k p_k^T),
\]

(36)

where \( P_k = \text{diag}\{p_k\} \). Therefore, the vector \( \bar{n} \) satisfies

\[
\mathbb{E}\{\bar{n}\} = 0, \quad \text{Cov}\{\bar{n}\} = \tilde{H} \text{Cov}\{\bar{p}_k\} \tilde{H},
\]

(37)

since the sign vector \( s_k \) does not have an effect on the covariance matrix. Thus we have the following results for \( \bar{c}_k \):

\[
\mathbb{E}\{\bar{c}_k\} = 1,
\]

\[
\text{Cov}\{\bar{c}_k\} = \|\alpha_k\|^2_1 \cdot \text{Cov}\{c_k \odot \bar{n}\}
\]

(38)

\[
= \frac{1}{N_s} \tilde{H} (P_k - p_k p_k^T) \tilde{H} \odot c_k c_k^T.
\]

For simplicity of further derivation, we use the notation of \( \mathbb{E}_k := \text{Cov}\{\bar{c}_k\} \).

### D. Error Scaling in the Presence of Monte Carlo-based QEM

In this subsection, we investigate the scaling law of computational error when the quantum circuit is protected by Monte Carlo-based QEM, based on the above discussions concerning the residual channels in the previous subsection.

We note that for QEM-protected circuits, the computational result is a random variable due to the randomness in the sampling procedure, given by

\[
r = v^T_{k-1} v_{N_G},
\]

(39)

where

\[
v_k = R_k v_0 = \bar{c}_k G_k v_{k-1}.
\]

(40)
After defining these quantities, we may obtain the following bound on the RMSE of the computational result \( r \).

**Proposition 3 (Square-root Increase of QEM Inaccuracy):** For a quantum circuit consisting of \( N_G \) gates which is protected by QEM, the RMSE of the computational result is upper bounded by

\[
\sqrt{\mathbb{E}\{(r - \tilde{r})^2\}} \leq 2^{n/2} \sqrt{\exp(2N_G N_s^{-1}) - 1}. \tag{41}
\]

This result is not restricted to Pauli channels. In fact, it applies to all completely positive trace-preserving channels, when the basis operators \( \{O_i\}_{i=1}^r \) are all completely positive trace-nonincreasing operators.

**Proof:** Please refer to Appendix [III] for the proof of this proposition, as well as additional discussions on Pauli channels as a special case.

Note that by applying the Taylor expansion to \( \exp(2N_G N_s^{-1}) \), we have

\[
\exp(2N_G N_s^{-1}) - 1 = \frac{2}{N_a} N_G + 1 - \frac{2}{N_a} N_G + \cdots,
\]

which is approximately \( 2N_G N_s^{-1} \), when \( N_G \ll N_s \). This means that when the RMSE is far less than 1, its scaling law is given by \( O(\sqrt{N_G}/\sqrt{N_s}) \). This is particularly useful, since in typical applications (e.g., variational quantum algorithms), having an RMSE close to 1 would be excessive.

In Proposition 3, the dependence of the RMSE on the error probability of quantum gates is not demonstrated. According to [91] of the Appendix, for Pauli channels, this dependence mainly relies on the term \( \| \Xi_k \|_{\text{max}} \). Next we expound a little further on this issue based on Assumption [I].

**Proposition 4 (Improved Bound for Pauli Channels):** Under Assumption [I] we have the following refined upper-bound for the RMSE of the computational result under Pauli channels:

\[
\sqrt{\mathbb{E}\{(r - \tilde{r})^2\}} \leq \frac{1}{2} \sqrt{\exp(\frac{1}{2} N_G N_s^{-1}) - 1} \tag{42}
\]

where \( \tilde{r} \) is given by

\[
\tilde{r} := \frac{5}{2} \sigma_a + \frac{1}{4} \sigma_a^2, \tag{43}
\]

and

\[
\sigma_a := 4 \epsilon u \cdot \frac{1 - \epsilon u}{(1 - 2 \epsilon u)^2}. \tag{44}
\]

The approximation is valid when \( \epsilon u \ll 1 \).

**Proof:** Please refer to Appendix [IV].

Verification of the approximation in (42) is straightforward: one may simply substitute (43) and (44) into (42). This proposition implies that, when \( \epsilon u N_G \ll N_s \), the RMSE is on the order of \( O(\sqrt{\epsilon u N_G}/\sqrt{N_s}) \).

Engendered by our specific proof technique, the factor \( 2^{n/2} \) in (41) and (42) seems to be an artifact. According to the numerical results which will be presented in Section [VI] we conjecture this factor is essentially unnecessary, implying that

\[
\sqrt{\mathbb{E}\{(r - \tilde{r})^2\}} \leq \sqrt{\exp(\epsilon N_G N_s^{-1}) - 1}. \tag{45}
\]

Regrettfully, it seems to be technically challenging to remove this factor from the bounds. Further investigations into this issue will be left for our future research.

---

Fig. 3. Schematic illustration of the Bloch sphere undergoing a sequence of imperfect single-qubit gates. The Bloch sphere shrinks when QEM is not applied, whereas it becomes “blurred” when the Monte Carlo-based QEM is applied.

V. DISCUSSIONS

A. Intuitions about the Error Scaling with the Circuit Size

As indicated by the results in Section [IV] with respect to \( N_G \), we observe an \( O(\sqrt{N_G}) \) scaling of the computational error of circuits protected by Monte Carlo-based QEM, when the number of samples is the same as that of QEM based on exact channel inversion. By contrast, when QEM is not applied, the computational error scales as \( O(N_G) \), as discussed in Section [IV]. Thus we may conclude that, although there are residual channels due to the inexact channel inversion, Monte Carlo-based QEM can still slow down the accumulation of computational error.

Revisiting the low-complexity example of a single-qubit circuit, we may understand these error scaling behaviours more intuitively. Specifically, the entire space of all legitimate single-qubit quantum states can be described by the celebrated Bloch sphere [35, Sec. 1.2]. As demonstrated in Fig. 3, the Bloch sphere would shrink as \( N_G \) increases when no QEM is applied, since the completely positive trace-preserving quantum channels are contractive transformations. This is in stark contrast with the case where Monte Carlo-based QEM is applied, when the Bloch sphere becomes “blurred” as \( N_G \) increases, since it is not determined whether the sphere will expand or shrink after each gate. Consequently, the sphere may expand after one gate and then shrink after another, hence the corresponding computational errors would cancel each other to a certain extent.

In light of the aforementioned intuition, we may interpret the error scaling of Monte Carlo-based QEM in following informal way. Assume that every gate \( k \) would transform the Bloch sphere in a way that its radius becomes \( (1 + \lambda_k) \) times that of its original value, where \( \lambda_k \) is a zero-mean random
C. The Intrinsic Uncertainty of the Computational Results

In the previous discussions, we followed the definition of computational results in (5). But even if the gates are decoherence-free, the intrinsic uncertainty of quantum states may bring some randomness to the computational result. To be specific, for a quantum state \( \rho \), the variance of a quantum observable \( O \) may be computed as follows [13]:

\[
\text{Var}_\rho(O) = \text{Tr}(O^2 \rho) - (\text{Tr}(\rho))^2,
\]

which quantifies the intrinsic uncertainty of the state \( \rho \) under the observable \( O \). If the quantum circuit is executed \( N_s \) times, the variance is then given by \( N_s^{-1} \text{Var}_\rho(O) \), and hence the mean-squared error (MSE) may be expressed as

\[
\text{MSE} = (r - \bar{r})^2 + \frac{1}{N_s} \cdot \text{Var}_\rho(O).
\]

We first consider the case where QEM is not applied. Since in VQAs, the observable \( \mathcal{M}_{\text{ob}} \) is typically implemented using a Pauli operator decomposition, its variance may also be decomposed as

\[
\text{Var}_{\rho|\mathcal{M}_{\text{ob}}} \{ \mathcal{M}_{\text{ob}} \} = \sum_{i=1}^{4^n} \frac{1}{2^n} |v_{\text{ob}}|^2 \text{Var}_{\rho|\mathcal{M}_{\text{ob}}} \{ S_i \}.
\]

We will therefore consider the case where QEM is applied. Note that in this case, the error scaling is as beneficial as that of the family of non-QEM-based solutions.
Hence
\[ \text{Var}_{\rho_{NG}} \{ \mathcal{M}_{ob} \} = \sum_{i=1}^{4^n} \frac{1}{2^n} |v_{ob}|^2 \left( 1 - (\text{Tr} \{ S_i \rho_{NG} \})^2 \right) \]
\[ = v_{ob}^T \left( \frac{1}{2^n} I - V_{NG} \right) v_{ob}, \]
where \( V_{NG} = \text{diag} \{ v_{NG} \} \). Note that from (7) we have \( |v_{NG}|^2 \leq 2^{-n} \) for all \( i \), hence it follows that
\[ 0 \leq \text{Var}_{\rho_{NG}} \{ \mathcal{M}_{ob} \} \leq 1. \]  
Thus the MSE of the computational result is bounded by
\[ (r - \overline{r})^2 \leq \text{MSE} \leq (r - \overline{r})^2 + \frac{1}{N_s}. \]  

When circuits are protected by QEM, it has been shown that [31] if the number of effective executions is \( N_s \), the variance equals to that in the case where QEM is not applied. Thus the total error scales on the order of
\[ O \left( \sqrt{\frac{\epsilon N_G}{N_s}} \right) + O \left( \sqrt{\frac{1}{N_s}} \right). \]  
This implies that, the effect of QEM may not be very significant when \( \epsilon N_G \ll 1 \). But note that when \( \rho_{NG} \) corresponds to one of the eigenstates of all Pauli operators \( i \) having non-zero coefficient \( |v_{ob}| \), we have
\[ \text{Var}_{\rho_{NG}} \{ S_i \} = 1 - (\text{Tr} \{ S_i \rho_{NG} \})^2 = 0, \]
which follows from that fact that Pauli operators only have eigenvalues of \( \pm 1 \). Therefore, QEM would be more effective when the final state \( \rho_{NG} \) is close to one of these eigenstates.

VI. Numerical Results

In this section, we evaluate the analytical results presented in the previous sections via numerical examples. If not otherwise stated, the following parameters and assumptions will be used throughout the section.
- The number of effective circuit executions is \( N_s = 5000 \);
- For Monte Carlo-based QEM, we use the same number of samples (i.e., actual circuit executions) as that of QEM based on exact channel inversion;
- The quantum channels modelling the gate imperfections are single-qubit depolarising channels having gate error probability \( 10^{-3} \).

A. Rotations Around the Bloch Sphere

We first consider the simplest scenario, where the quantum circuits are constituted of single-qubit gates, because these simple circuits allow us to clearly observe the error scaling described in the previous sections. In particular, we consider the circuits shown in Fig. 5. The quantum observable \( \mathcal{M}_{ob} \) in this example is the Pauli Z operator \( Z \) on the qubit, which satisfies
\[ Z |0\rangle = |0\rangle, \quad Z |1\rangle = -|1\rangle. \]
The corresponding PTM representation is given by \( v_{ob} = [0 0 0 \sqrt{2}]^T \).
inversion scales as $O(\sqrt{N_G})$ for small $N_G$, but converges to a constant ($\approx \sqrt{N_s^{-1}}$) when $N_G$ is large. Furthermore, when $N_G$ is large, the RMSE of circuits operating without QEM protection converges to a constant. This agrees with Proposition 1 which indicates that their computational results converge to zero regardless of the quantum observable.

The RMSE scalings with respect to the gate error probability $\epsilon$ are shown in Fig. 6b where we choose $N_G = 10$, while the number of effective circuit executions, namely $N_s = 5000$, does not vary as the gate error probability increases. It is noteworthy that when $\epsilon$ is small, the RMSE of circuits operating without QEM protection is lower than that of their counterparts protected by QEM. This phenomenon may be understood from our discussion in Section V-B where we have indicated that the error scaling of QEM-protected circuits is $O(\epsilon N_{G}^{-1})$. Compared to the $O(\epsilon)$ scaling of non-QEM-protected circuits, the RMSE may be higher when $\epsilon$ is much smaller than $N_G$. Interestingly, as seen from the figure, the square root scaling with respect to $\epsilon$ becomes preferable to the linear scaling when $\epsilon$ is relatively large.

For the circuit comprising repeated rotations around the $X$-axis, as illustrated in Fig. 5 we set $\theta = \pi/256$, and the results are plotted in Fig. 7. Observe that the envelope of the RMSE curves exhibit similar scaling behaviours as those in Fig. 6b but there are some oscillations. To understand the RMSE oscillations of circuits protected by Monte Carlo-based QEM, from (90) we may express the covariance matrix of $v_k$ as follows

$$
\Sigma_k = (1^T + \Xi_k) \otimes G_k \Sigma_{k-1} G_k^\dagger + \Xi_k \otimes \mu_k \mu_k^T.
$$

(53)

Note that the term $\Xi_k \otimes \mu_k \mu_k^T$ varies with $k$ under the observable $\mathcal{M}_{\text{obs}} = Z$, and hence the RMSE is oscillatory.

The RMSE oscillation of non-QEM-protected circuits may be better understood by investigating the evolution of the computational result $r$ as $N_G$ increases, which is portrayed in Fig. 8. It can be seen that the mean values of the non-QEM-protected circuits fit nicely within the bounds given by Proposition 1. Furthermore, the RMSE of QEM-protected circuits is mainly contributed by the variance of the computational results, while the RMSE of circuits not protected by QEM is mainly determined by the mean value, since in the latter case the bias is far larger than the standard deviation. As the dynamic range of the mean values is reduced, by coincidence, there are multiple intersections of the ground truth and the mean values, and thus the computational error of non-QEM-protected circuits oscillates as $N_G$ increases.

Finally, we demonstrate that some non-Pauli channels may also exhibit the $O(\sqrt{N_G})$ error scaling. In particular, we consider amplitude damping channels [39] having the following PTM representation

$$
C_{\text{damp}} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \sqrt{1-\gamma} & 0 & 0 \\
0 & 0 & \sqrt{1-\gamma} & 0 \\
\gamma & 0 & 0 & 1-\gamma
\end{pmatrix},
$$

(54)

where $\gamma$ is the amplitude damping probability. Here, we set the amplitude damping probability to $\gamma = 1 \times 10^{-3}$. The RMSE scalings with respect to the number of gates $N_G$ are shown in Fig. 9a for the circuit comprising repeated Pauli X gates, and in Fig. 9b for the circuit consisting of repeated ($\pi/256$) rotations around the $X$-axis. We observe that the curves corresponding to QEM based on exact channel inversion and those corresponding to Monte Carlo-based QEM exhibit the $O(\sqrt{N_G})$ scaling behavior, while the non-QEM-protected curves scale as $O(N_G)$, which is similar to the error scaling behaviour under Pauli channels as portrayed in Fig. 6 and Fig. 7.

**B. The Quantum Approximate Optimization Algorithm Aided Multi-User Detection**

In this subsection, we apply our analytical results to a practical variational quantum algorithm, the quantum approximate optimization algorithm [14], which aims for solving
combinatorial optimization problems assuming the following form
\[
\max_{\mathbf{z} \in \{-1, +1\}^n} \sum_{k=1}^{K} w_k \prod_{i=1}^{n} z_{k,i},
\]
where \( \mathbf{z} = [z_1 \ldots z_n]^T \), and \( l_{k,i} \in \{1, 2, \ldots, n\} \). In the formulation of the quantum approximate optimization algorithm, the problem (55) is transformed into the maximization of \( \langle \psi | \mathcal{H} | \psi \rangle \), where the quantum observable \( \mathcal{H} \) is given by
\[
\mathcal{H} = \sum_{k=1}^{K} w_k \prod_{i=1}^{n} Z_{l_{k,i}}.
\]
The trial state \( |\psi\rangle \) is prepared using a parametric circuit having an alternating structure, so that
\[
|\psi\rangle = e^{-i\beta_P B} e^{-i\gamma_P \mathcal{H}} \ldots e^{-i\beta_1 B} e^{-i\gamma_1 \mathcal{H}} |\rangle^{\otimes n},
\]
where \( P \) is the number of stages in the alternating circuit, and \( B \) is the “mixing Hamiltonian” [17] given by \( B = \sum_{i=1}^{n} \lambda_i \). The parameters \( \beta = [\beta_1 \ldots \beta_P]^T \) and \( \gamma = [\gamma_1 \ldots \gamma_P]^T \) are typically obtained using via an optimization procedure implemented on classical computers [12]. For the purpose of this treatise, here we do not optimize the parameters, but use the following (suboptimal) adiabatic configuration [40] instead
\[
\gamma_k = kP^{-1}, \quad \beta_k = 1 - kP^{-1}.
\]

We consider the multiuser detection problem of wireless communications [41]. In particular, assuming that the modulation scheme is BPSK, in a spatial division multiple access system, the signal received at a base station equipped with \( m \) antennas from \( n \) single-antenna uplink transmitters may be expressed as
\[
\mathbf{y} = \mathbf{H} \mathbf{x} + \mathbf{w},
\]
where \( \mathbf{H} \in \mathbb{R}^{m \times n} \) denotes the channel, \( \mathbf{x} \in \{-1, +1\}^n \) represents the transmitted signal, and \( \mathbf{w} \in \mathbb{R}^m \) is the noise. We assume here that the noise is i.i.d. Gaussian. Hence the maximum likelihood estimate of \( \mathbf{x} \) is given by
\[
\hat{\mathbf{x}}_{\text{ML}} = \arg \max_{\mathbf{x} \in \{-1, +1\}^n} 2(\mathbf{H}^\dagger \mathbf{y})^\dagger \mathbf{x} - \mathbf{x}^\dagger \mathbf{H}^\dagger \mathbf{H} \mathbf{x}.
\]
This may be further reformulated as the maximization of the quadratic form \( \langle \psi | \mathcal{H} | \psi \rangle \), where
\[
\mathcal{H} = \frac{1}{Z} \left( \sum_{i=1}^{n} [\mathbf{H}^\dagger \mathbf{y}]_i Z_i - \sum_{i=1}^{n} \sum_{j=i+1}^{n} [\mathbf{H}^\dagger \mathbf{H}]_{i,j} Z_i Z_j \right),
\]
and \( Z \) is a normalizing coefficient ensuring that the quantum observable \( \mathcal{H} \) satisfies our Assumption 2.

In this illustrative example, we consider the case where \( m = n = 4 \). For the entries of the channel \( \mathbf{H} \) are i.i.d. Gaussian variables with zero mean and variance \( m^{-1} \) [42]. For the quantum circuits, we choose gate error probability \( \epsilon = 3 \times 10^{-4} \). Under these assumptions, the RMSE scalings with respect to \( P \) of non-QEM-protected circuits and that of circuits protected by Monte Carlo-based QEM are portrayed in Fig. 10. It can be observed that the non-QEM-protected circuits exhibit an \( O(P) \) scaling, while the QEM-protected circuits exhibit an \( O(\sqrt{P}) \) scaling, as indicated by Propositions 2 and 4 respectively.

To illustrate the evolution of the computational results during the execution of circuits, we plot the objective function values (i.e., \( \langle \psi | \mathcal{H} | \psi \rangle \)) computed at each stage \( k \) of the circuits in Fig. 11 for the case where \( P = 225 \). Note that the results computed by the QEM-protected circuits converge monotonically towards the optimum, for which the main source of error is the variance. By contrast, for the non-QEM-protected circuits, the results were on the right track for \( k < 100 \), but soon they deviate from their QEM-protected counterparts, and start to converge to zero. In this example, the bound (25) is not as tight as it was in Section VI.A but it still indicates that the dynamic range of the results computed by non-QEM-protected circuits decays exponentially as \( k \) increases.

VII. CONCLUSIONS

The trade-off between the computational overhead and the error scaling behaviour of both quantum circuits protected
by Monte Carlo-based QEM and their non-QEM-protected counterparts was investigated. As for the non-QEM-protected circuits, we have shown that the dynamic range of the noisy computational results shrinks exponentially as the number of gates \( N_G \) increases, implying a linear error scaling with \( N_G \). By contrast, the error scales as the square root of \( N_G \) in the presence of Monte Carlo-based QEM, at the same computational cost as that of QEM based on exact channel inversion. Moreover, the error scaling of Monte Carlo-based QEM can be further improved with increased computational cost.

We have also demonstrated the analytical results both for low-complexity examples and for a more practical example of the quantum approximate optimization algorithm employed for multi-user detection in wireless communications. It may be an interesting future research direction to apply the results to other practical examples, or verify them using experimental approaches.

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APPENDIX I

PROOF OF PROPOSITION 1

Proof: First observe that the matrix representation of a perfect gate \( G_i \) as well as that of a channel \( C_i \) take the following block-diagonal form

\[
G_i = \begin{pmatrix} 1 & 0^T \\ 0 & U_i \end{pmatrix}, \quad C_i = \begin{pmatrix} 1 & 0^T \\ 0 & D_i \end{pmatrix},
\]

(58)

where \( U_i \) is a unitary matrix, whereas \( D_i \) is a diagonal matrix having diagonal entries taking values in the interval \([0,1]\). Since the matrix \( R_{N_G} \) is the product of several \( G_i \) and \( C_i \), it becomes clear that its largest singular values satisfies \( \sigma_1(R_{N_G}) = 1 \), and its second largest singular value satisfies

\[
\sigma_2(R_{N_G}) \leq \prod_{i=1}^{N_G} \|D_i\|_2.
\]

(59)

Furthermore, we have

\[
\left| r - \frac{1}{2n} \text{Tr} \{M_{\text{obs}}\} \right| \leq \sigma_2(R_{N_G})
\]

(60)

due to the “bounded observable” Assumption 2.

Note that the quantity \( N_L \) defined in this proposition is related to the depth of the circuit. To elaborate, if we say that “a layer of gates” is executed if each qubit has been processed by at least one gate, then the entire circuit consists of at least \( N_L \) layers. For each single-qubit channel \( C \) in these layers, due to the assumption that each single-qubit Pauli error occurs at probability of at least \( \epsilon_1 \), the following bound holds:

\[
C = I - 2\text{diag} \{p_X + p_Z, p_Y + p_Z, p_X + p_Y\} \leq (1 - 4\epsilon_1),
\]

(61)

where \( p_X, p_Y \) and \( p_Z \) are error probabilities corresponding to the Pauli-X, Y and Z errors, respectively. Thus we obtain

\[
\sigma_2(R_{N_G}) \leq (1 - 4\epsilon_1)^{N_L} = \exp\{N_L \ln(1 - 4\epsilon_1)\}
\]

(62)

\[
\leq \exp(-4\epsilon_1 N_L).
\]

Hence the proof is completed.

APPENDIX II

PROOF OF PROPOSITION 3

Proof: In this proof, we will work under the operator-sum representation of quantum channels. Since we consider Pauli channels, the recursion (3) may be rewritten as

\[
\rho_k = \sum_{i=1}^{4^n} |p_k_i\rangle S_i G_k \rho_{k-1} G_k^\dagger S_i
\]

(63)

\[
= |p_k| S_i G_k \rho_{k-1} G_k^\dagger + \sum_{i=2}^{4^n} |p_k_i\rangle S_i G_k \rho_{k-1} G_k^\dagger S_i.
\]
Assumption \[2\] implies that \(\|M_{ob}\|_2 \leq 1\), meaning that
\[\text{Tr} \{M_{ob}\rho\} \leq 1\]
holds for any legitimate density matrix \(\rho\). Note that terms such as \(S_i G_k \rho_{k-1} G_j S_i\) in (63) are indeed legitimate density matrices. Thus the computational result satisfies
\[|\bar{r} - \text{Tr} \{M_{ob}\rho_{NG}\}| \leq (|\bar{r}| + \|M_{ob}\|_2) \left(1 - \prod_{k=1}^{N_G} |p_k|_1\right) \leq 2 \left(1 - \prod_{k=1}^{N_G} |p_k|_1\right).
\]
According to Assumption \[1\] for any \(k\), the vector \(p_k\) satisfies
\[|p_k|_1 \geq 1 - \epsilon_u,
\]
\[\sum_{i=2}^{4^n} |p_k|_i \leq \epsilon_u.
\]
Therefore, we have
\[|\bar{r} - \text{Tr} \{M_{ob}\rho_{NG}\}| \leq 2(1 - (1 - \epsilon_u)^{N_G}) \leq 2\epsilon_u N_G.
\]
Hence the proof is completed.

\[\square\]

**APPENDIX III**

**PROOF OF PROPOSITION \[3\]**

*Proof:* We first expand the expression of MSE as follows
\[\mathbb{E}\{(r - \bar{r})^2\} = \mathbb{E}\left\{(v_{ob}^T \nu_{NG} - \bar{r})^2\right\} = v_{ob}^T \mathbb{E}\{\nu_{NG} \nu_{NG}^T\} v_{ob} + \bar{r}^2 - 2\bar{r} v_{ob} \mathbb{E}\{\nu_{NG}\}.
\]
Hence the RMSE is given by
\[\sqrt{\mathbb{E}\{(r - \bar{r})^2\}} = \sqrt{v_{ob}^T A_k v_{ob} + \bar{r}^2 - 2\bar{r} v_{ob} \mathbb{E}\{\nu_{NG}\},
\]
where \(A_k := \mathbb{E}\{v_k v_k^T\}\) and \(\mu_k := \mathbb{E}\{v_k\}.
\] Using (32) and (40), we have
\[v_k = \sum_{i=1}^L [\alpha_k]_i O_i C_k G_k v_{k-1}.
\]
This implies the following recursive relationships:
\[A_k = \sum_{i=1}^L \sum_{j=1}^L e_{ij}^{(k)} O_i C_k G_k A_{k-1} G_k^T C_k^T O_j^T,\]
\[\mu_k = G_k \mu_{k-1},\]
where \(e_{ij}^{(k)} = |E_{ij}|_{ij} := \mathbb{E}\{[\alpha_k]_i [\alpha_k]_j\}\). The matrix \(E_k\) may be expressed as
\[E_k = \mathbb{E}\{\bar{E}_k\} = \alpha_k \alpha_k^T + ||\alpha_k||_2^2 \text{Cov}\{\bar{p}_k\},
\]
\[= \alpha_k \alpha_k^T + \frac{1}{N_s} (P_k - \bar{p}_k \bar{p}_k^T).
\]
For the simplicity of further derivation, we denote \(\bar{E}_k := \frac{1}{N_s} (P_k - \bar{p}_k \bar{p}_k^T)\).

Let us now consider the case of \(k = 1\). In this case, \(v_0\) of (8) is a deterministic vector, thus we have
\[A_0 = v_0 v_0^T,\]
\[\mu_0 = v_0\]

Using the recursive relationship of \(\mu_k = G_k \mu_{k-1}\), we now see that \(v_{ob}^T \mu_{NG} = \bar{r}\). Hence we may simplify (67) as
\[\mathbb{E}\{(r - \bar{r})^2\} = v_{ob}^T \Sigma_k v_{ob} + \bar{r}^2 - 2\bar{r} v_{ob} \mathbb{E}\{\nu_{NG}\}.
\]
The covariance matrix can be further formulated as
\[\Sigma_k = A_k - \mu_k \mu_k^T = A_k - R_k v_0 v_0^T R_k^T.
\]
It now suffices to compute \(A_k\). Taking trace from both sides of (70a), we have
\[\text{Tr} \{A_k\} = \sum_{i=1}^L \sum_{j=1}^L e_{ij}^{(k)} \text{Tr} \{O_i C_k G_k A_{k-1} G_k^T C_k^T O_j^T\}.
\]
Next we consider the decomposition
\[e_{ij}^{(k)} = [\alpha_k]_i [\alpha_k]_j + [\bar{E}_k]_{ij}.
\]
Observe that the term \(A_{NG} - \mu_{NG} \mu_{NG}^T\) is in fact the covariance matrix of \(\nu_{NG}\), upon defining
\[\Sigma_k := A_k - \mu_k \mu_k^T.
\]
and substituting into (72) we arrive at
\[\mathbb{E}\{(r - \bar{r})^2\} = v_{ob}^T \Sigma_k v_{ob}.
\]
(75)

The covariance matrix can be further formulated as
\[\Sigma_k = A_k - \mu_k \mu_k^T = A_k - R_k v_0 v_0^T R_k^T.
\]
(76)

where the third line follows from the fact that all the basis operators \(O_i, i = 1 \ldots L\) are trace-nonincreasing operators, hence represent contractive transformations. Since unitary transformations preserve the trace, we further obtain
\[\text{Tr} \{A_k\} \leq \text{Tr} \{A_{k-1}\} (1 + \lambda_{\text{max}} \{C_k^T C_k\} \sum_{i=1}^L \sum_{j=1}^L [\bar{E}_k]_{ij})\]
(81)
Note that

\[ \sum_{i=1}^{L} \sum_{j=1}^{L} [E_k]_{ij} \leq \frac{1}{N_s} \left( \| \text{vec}(P_k) \|_1 + \| \text{vec}(p_kp_k^T) \|_1 \right) \]

= \frac{2}{N_s}, \tag{82}

and that \( \lambda_{\max} \{ C_k^T C_k \} \leq 1 \) since \( C_k \) is a completely positive trace-preserving channel, hence is contractive. In light of this, the upper bound of \( \text{Tr} \{ A_k \} \) can now be simplified as follows:

\[ \text{Tr} \{ A_k \} \leq \text{Tr} \{ A_{k-1} \} \left( 1 + \frac{2}{N_s} \right). \tag{83} \]

From (72) we have \( \text{Tr} \{ A_0 \} = 1 \) since \( v_0 \) is a unit vector, hence we obtain

\[ \text{Tr} \{ A_{N_G} \} \leq \prod_{k=1}^{N_G} \left( 1 + \frac{2}{N_s} \right) \leq \exp \left( 2N_GN_s^{-1} \right). \tag{84} \]

Using (76), we have

\[ \text{Tr} \{ \Sigma_{N_G} \} = \text{Tr} \{ A_{N_G} \} - \text{Tr} \{ v_0v_0^T \} \leq \exp \left( 2N_GN_s^{-1} \right) - 1. \tag{85} \]

Note that \( \Sigma_{N_G} \) is a positive semidefinite matrix, hence we have

\[ \text{Tr} \{ \Sigma_{N_G} \} \geq \lambda_{\max}(\Sigma_{N_G}), \tag{86} \]

where \( \lambda_{\max}(\cdot) \) denotes the maximum eigenvalue of a matrix. This implies that

\[ \sqrt{\mathbb{E} \{ (r-\bar{r})^2 \}} \leq \sqrt{\text{Tr} \{ \Sigma_{N_G} \}} \cdot \| v_{ob} \| \leq \sqrt{\exp \left( 2N_GN_s^{-1} \right) - 1} \cdot \| v_{ob} \|. \tag{87} \]

Hence the proof is completed by applying (23). \( \square \)

Especially, for Pauli channels, we have the following simplified recursions:

\[ A_k = \mathbb{E} \{ \bar{c}_k \bar{c}_k^T \} \circ G_k A_{k-1} G_k^T, \tag{88} \]

\[ \mu_k = G_k \mu_{k-1}. \]

In fact, we have

\[ \mathbb{E} \{ \bar{c}_k \bar{c}_k^T \} = 11^T + \Xi_k, \tag{89} \]

which follows from (38). Substituting (89) into (88), we obtain

\[ A_k = G_k A_{k-1} G_k^T + \Xi_k \circ G_k A_{k-1} G_k^T. \tag{90} \]

Following the same line of reasoning as we used in the general case, we have

\[ \text{Tr} \{ A_k \} = \text{Tr} \{ G_k A_{k-1} G_k^T + \Xi_k \circ G_k A_{k-1} G_k^T \} \]

\[ = \text{Tr} \{ A_{k-1} \} + \text{Tr} \{ \Xi_k \circ G_k A_{k-1} G_k^T \} \]

\[ \leq \text{Tr} \{ A_{k-1} \} \left( 1 + \| \Xi_k \|_{\max} \right), \tag{91} \]

the “max norm” \( \| \cdot \|_{\max} \) is defined as

\[ \| A \|_{\max} := \max_{i,j} |A_{i,j}|. \]

From (38) we obtain

\[ \| \Xi_k \|_{\max} = \frac{1}{N_s} \| \tilde{H} (P_k - p_k p_k^T) \tilde{H} \circ c_k c_k^T \|_{\max} \]

\[ \leq \frac{1}{N_s} \| \tilde{H} (P_k - p_k p_k^T) \tilde{H} \|_{\max} \| c_k c_k^T \|_{\max} \tag{92} \]

\[ \leq \frac{1}{N_s} \left( \| \tilde{H} P_k \tilde{H} \|_{\max} + \| \tilde{H} p_k p_k^T \tilde{H} \|_{\max} \right), \]

where the third line follows from the fact that \( c_k \) represents a contractive transformation, so that \( c_k \leq 1 \). Note that every entry in \( \tilde{H} \) has an absolute value of 1, and hence

\[ \| \tilde{H} P_k \tilde{H} \|_{\max} \leq \| \text{vec}(P_k) \|_1 = 1, \tag{93} \]

and

\[ \| \tilde{H} p_k p_k^T \tilde{H} \|_{\max} \leq \| \text{vec}(p_k p_k^T) \|_1 = 1. \tag{94} \]

Hence we arrive at exactly the same bound as given in (87).

**APPENDIX IV**

**PROOF OF PROPOSITION 4**

**Proof:** We start the proof from revisiting the inequality in (22), and arrive at:

\[ \| \Xi_k \|_{\max} \leq \frac{1}{N_s} \| \tilde{H} (P_k - p_k p_k^T) \tilde{H} \|_{\max} \]

\[ \leq \frac{1}{N_s} \| \text{vec}(P_k - p_k p_k^T) \|_1. \tag{95} \]

Next we construct an upper bound for the term \( \| \text{vec}(P_k - p_k p_k^T) \|_1 \). According to the sampling overhead of QEM in [22], Assumption 1 implies that

\[ \| \alpha \|_1 \leq \sqrt{1 + \sigma_a}. \tag{96} \]

Since \( \alpha_k^{(1)} \geq 1 \), we have

\[ \sum_{i \neq 1} |\alpha_k^{(i)}| \leq \sqrt{1 + \sigma_a} - 1. \tag{97} \]

This further implies that

\[ p_k^{(1)} \geq \frac{1}{\sqrt{1 + \sigma_a}}, \tag{98} \]

\[ \sum_{i \neq 1} p_k^{(i)} \leq \sqrt{1 + \sigma_a} - 1. \]

Therefore, upon taking the entry-wise absolute value, we obtain

\[ |P_k - p_k p_k^T| \leq \left( \begin{array}{cccc} \frac{\sigma_a}{1 + \sigma_a} & p_k^{(2)} & \cdots & p_k^{(4^n)} \\ \frac{\sigma_a}{1 + \sigma_a} & p_k^{(2)} & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sigma_a}{1 + \sigma_a} & \vdots & \cdots & p_k^{(4^n)} \end{array} \right). \tag{99} \]

Here, the symbol “\( \leq \)” stands for entry-wise “not larger than”. Observe that summing up the first row, the first column and the main diagonal, by applying (98), we see that

\[ \| \text{vec}(P_k - p_k p_k^T) \|_1 \leq 3 \sqrt{1 + \sigma_a} - 1 + \frac{\sigma_a}{1 + \sigma_a} + \| \text{vec}(q_k q_k^T) \|_1, \tag{100} \]

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where $q_k := \left[p_k^{(2)} \ldots p_k^{(4)}\right]^T \in \mathbb{R}^{4^{k-1}}$. Note that
\[
\left\|\text{vec}\{q_k q_k^T\}\right\|_1 = 1^T q_k q_k^T 1 \leq (\sqrt{1 + \sigma_u} - 1)^2,
\]
(101)

implying that
\[
\left\|\text{vec}\{P_k - p_k p_k^T\}\right\|_1 \leq \frac{5}{2} \sigma_u + \frac{1}{4} \sigma_u^2,
\]
(102)

which follows from that fact that
\[
\sqrt{1 + x} - 1 \leq \frac{x}{2}
\]
holds for all $x \geq 0$. Hence we have
\[
\|\mathcal{E}_k\|_{\max} \leq \frac{1}{N_8} \left(\frac{5}{2} \sigma_u + \frac{1}{4} \sigma_u^2\right),
\]
(103)

which proves (42). Thus the proof is completed.

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