I. INTRODUCTION

Detection and diagnosis of faults in classical digital circuits have been part of mainstream circuit manufacturing research and industry for several decades. A common approach for this is to analyze outputs when a circuit is given a fixed set of carefully chosen inputs (also known as patterns). ATPG (automated test pattern generation) techniques essentially try to efficiently generate an effective set of such inputs. This is computationally challenging because it belongs to the category of NP-complete problems [1]. However, extremely efficient heuristics have led to successful adoption of ATPG in VLSI.

ATPG is an obvious avenue to explore fault detection in quantum circuits; however, current results on ATPG for quantum circuits are few and do not seem to fully exploit the power of quantum computation in generating an efficient set of test patterns. In this regard, we noted the idea of quantum tomographic testing that has been discussed earlier in [2, 3]. Like quantum state tomography, quantum tomographic testing requires multiple measurements on the circuit in question on various inputs; the histogram or the frequency counts of output patterns can be used to approximately determine the output states. The pairs of input and output states are then analyzed to detect and diagnose faults in the circuit.

Theoretically the number of possible faults is endless for any quantum circuit. Practically however, a method of synthesizing a circuit limits the possible set of faults. Single fault assumption is now routine used in academia and industry in which the cause of a circuit failure is attributed to only one faulty component (gate). Hayes et al. reported that the commonly used “stuck-at” fault-model and “bridging fault-model are not very apt for quantum circuits [4]. They proposed the missing gate fault (MGF) model in which one or more quantum gates are missing, i.e., these gates behave like an identity operator. ATPG for quantum circuits have since then largely focused around single MGF (SMGF). It is of course clear that if a gate behaves almost like an identity operator, then detecting whether it is present or missing is going to be difficult, if not impossible. However, formal understanding of this statement was not available so far.

In this work we explain what it means for a gate to be hard to diagnose (maybe more computation is required but no faulty gate is impossible to diagnose). We further show how to efficiently obtain a set of input states and measurement operators to cover all faulty gates with much less trials compared to existing results [2, 3]. Unlike these works, our detailed explanations pertain to arbitrary single gate fault models, including SMGF; the faults may even be different for each gate. Furthermore, we do not require any internal modification of the circuit (unlike [3]).

The technical contribution is essentially answers to a set of questions raised, but left unaddressed, in [2]. Central to these are three observations, all of which are peculiarities of quantum circuits not present in their classical cousins. Suppose we have two states $|u\rangle$ and $|v\rangle$ whose output, when measured identically, generate the...
probability distributions \( \{ u_m \} \) and \( \{ v_m \} \), respectively, on measurement outcomes. The first observation is that the “difference” caused by faulty behaviour of any gate is preserved subsequently. In other words, statistical distance between \( \{ u_m \} \) and \( \{ v_m \} \) does not change if an identical quantum circuit is applied on both the states before measuring.

The second observation is that using the same measurement operators on some combination of the input states \( (\alpha |u\rangle + \beta |v\rangle) \) generates a probability distribution which is not a linear combination \( \{(\alpha^2 |u\rangle \langle u| + \beta^2 |v\rangle \langle v|) \} \) of the earlier probability distributions. Therefore, it makes sense to explicitly consider input states that are in superpositions of standard basis states.

Finally, motivated by the last reason, we ought to take advantage of the generalized measurement operators that quantum systems allow beyond the usual practice of measuring in the standard basis. It is therefore immediate that, unlike earlier approaches \([2, 3]\), we ought to be looking for input states that could be superposition of basis states, and measurement operators more general than projective measurements in the standard basis.

We will denote by \( C \) the circuit to be diagnosed which acts on \( n \) qubits and represent its gates when enumerated in the standard manner, by \( G_1, G_2, \ldots, G_s \). To simplify our explanation, we will say \( G_0 \) is fault-free to mean that \( C \) is fault-free. In the fault model we consider, at most one of these \( s \) gates is faulty, and when faulty, the corresponding faulty behaviour (operator) is known to us. The operators for the fault-free and faulty \( i \)-th gate are denoted by \( G^i \) and \( G_j^i \), respectively \((G_j^i \) is set to the identity operator under the SMGF model). Let \( C^0 \) denote a circuit in which no gate is faulty, and \( C^a \) denote a circuit in which (only) the \( i \)-th gate is faulty. That is, \( C^0 = G^s \ldots G^{i+1}G^iG^{i-1} \ldots G^1 \) and \( C^a = G^s \ldots G^{i+1}G_j^iG^{i-1} \ldots G^1 \). We want to detect if \( C \) is fault-free or faulty, and furthermore, if faulty then diagnose the offending gate; in other words, we want to know \( C = C^j \) for which \( j \in \{0, \ldots, s\} \). We illustrate the effectiveness of our strategy by applying it on a benchmark circuit “3qubitnot”.

II. DETECTING IF A SPECIFIC GATE IS FAULTY

This section contains the main tools of this paper. Suppose we are told that all but the \( i \)-th gate are fault-free. We want to detect if the \( i \)-th gate is fault-free or faulty. For the sake of brevity, we will use the following notation in this section: \( G = G^j, G_f = G_j^i \), \( C = C^0 \) and \( C^a = C^j \). Thus, we want to know if the \( i \)-th gate is \( G \) or \( G_f \).

The high-level idea of our approach is to

1. Find an input state \( |\phi\rangle \) such that \( |\psi\rangle = C |\phi\rangle \) and \( |\psi'\rangle = C^j |\phi\rangle \) are at the farthest “distance” possible.

2. Find measurement operators which can distinguish between those two faraway states \( |\psi\rangle \) and \( |\psi'| \) with minimal probability of failure.

The fact that these can be done in general is well-known \([4]\). We reformulate the known results and describe how to derive optimum input state and measurement operators to solve the problem described above.

A. Optimal input state

The appropriate measure of “distance” for pure quantum states with respect to distinguishability is the trace distance defined by \( D(|\psi\rangle, |\psi'|) = \sqrt{1 - |\langle \psi | \psi' \rangle|^2} \).

Trace distance is also equal to the maximum L1 distance of the probability distributions obtained from the two states upon measurement \([10]\). Given two operators \( G \) and \( G_f \), we say that a state \( |\phi\rangle \) is a \((G, G_f)\)-separator (similarly, \((C, C')\)-separator) if this state, given as input, maximizes the trace distance between \( G |\phi\rangle \) and \( G_f |\phi\rangle \) (respectively, \( C |\phi\rangle \) and \( C' |\phi\rangle \)).

Therefore, our immediate goal is to find a \((C, C')\)-separator input state \( |\phi\rangle \) which minimizes \( |\langle \psi | \psi' \rangle| \). Our main observation here is that we can decompose our circuits into common sub-circuits excluding the \( i \)-th gate: \( C = C_2G_C1 \) and \( C' = C_2G_fC1 \). Let \( S = G^iG_f \). Without loss of generality, we can consider that \( G \) (hence, \( G' \) and \( S \)) acts on all \( n \) qubits (possibly by tensoring with an identity operator of suitable dimensions).

Let the the eigenvalues of \( S \) be denoted by \( e^{-i\theta_1}, \ldots, e^{-i\theta_m} \) (including duplicates) and the corresponding eigenvectors by \( |v_1\rangle, \ldots, |v_m\rangle \). Let \( \bar{a} = \{a_1 \ldots a_m\} \) be a solution to this optimization problem:

\[
\text{OPT} : \quad \min \sum_j a_j^2 + \sum_{j, k \neq i} a_j a_k \cos(\theta_j - \theta_k) \\
\text{subject to :} \quad \sum_j a_j = 1, \quad 0 \leq a_j \leq 1
\]

First observe that minimizing Eqn. 1 is equivalent to minimizing

\[
\left\lVert \sum_j a_j^2 + \sum_{j, k \neq i} a_j a_k \cos(\theta_j - \theta_k) \right\rVert
\]

where \( |\phi\rangle = \sum_j \sqrt{a_j} |v_j\rangle \) is a state on \( n \) qubits.

Therefore the optimum \( \bar{a} \) for \( \text{OPT} \) minimizes \( |\langle \phi' | G^iG_f | \phi' \rangle| \), which makes \( |\phi'\rangle \) a \((G, G_f)\)-separator.

We can now choose \( |\phi\rangle = C_1 |\phi'\rangle \) as our required \((C, C')\)-separator input. Since \( |\langle \phi' | S | \phi' \rangle| = |\langle \phi | C_2G_C1 | \phi \rangle| = |\langle \phi | C_1C' | \phi \rangle| = |\langle \psi | \psi' \rangle| \), the optimum \( \bar{a} \) also minimizes \( |\langle \psi | \psi' \rangle| \) and this minimum value is simply \( \sum_j a_j e^{-i\theta_j} \).
The above optimization problem is not a computational hurdle for three reasons. First, the number of variables is exponential only in the dimension of the gate involved, which is usually quite small in practice. Secondly, OPT has the form of an equality-constrained quadratic program for which efficient algorithms exist.

The final reason is the interesting fact that the separator input for a gate in a circuit depends fundamentally on the gate in question and corresponding fault model. It does not depend at all on the portion of the circuit coming after the faulty gate (C₂), and its dependence on the portion of the circuit before the faulty gate (C₁) is really incidental. Therefore, it is feasible to have a precomputed table of \((G, G_f)\)-separators for different gates under common fault models. The required separator input for any circuit can be obtained by running the first portion of the circuit in reverse on a gate-separator input. Quantum circuits are usually built using a small set of involved, which is usually quite small in practice. Secondly,\(^\text{57–9}\), a general design and implement measurement operators that are able to distinguish between these states. and thereby determine if the circuit in question is \(C\) or \(C'\). However, unlike input states, measurement operators depend on the actual circuit and has to be computed once for every circuit and every fault model.

The question of distinguishing between two given quantum states is one of the classical problems of quantum computing\(^\text{10}\). Two states can be differentiated (using measurements) with certainty if and only if they are orthogonal. So, if \(G_f\) is almost same as \(G\), then obviously no measurement should be able to distinguish between them with high confidence. We show below that we can distinguish with high confidence for gates with low value of \[ |\sum_j a_j e^{-i \theta_j}| \] (obtained by solving OPT).

There are two known modes of distinguishing between a pair of states. Helstrom measurement is a two-output (von Neumann) projective measurement which minimizes the error of incorrect labelling\(^\text{11}\). If we prohibit incorrect outcome and instead allow our measurement operators to either label a state with certainty or report “?” (inconclusive), then we would be performing what is known as unambiguous state discrimination (USD). USD is commonly achieved by employing a POVM\(^\text{7,12}\), a generalization of the Helstrom measurement. Table I presents the separator input states for various commonly used gates in the SMGF model.

---

**Table I. Optimal \((G, I)\)-separator inputs states \((|\phi'\rangle)\) and corresponding probability of error \((\delta)\) using optimal projective measurement operators for detecting missing quantum gates.**

| Gate  | Separator input states | Error prob. |
|-------|------------------------|-------------|
| Hadamard | \[ -\sqrt{2\pi} \] | 0.00 |
| Phase | \[ 1/\sqrt{2} \]  | 0.15 |
| \(C\text{NOT}\) | \[ \begin{pmatrix} 0.4082 \\ -0.2113 \\ 0.7887 \end{pmatrix} \] | 0.00 |
| \(R_y(\pi/6)\) | \[ \begin{pmatrix} 0 \\ -1 \end{pmatrix} \] | 0.37 |
| \(R_z(\pi/16)\) | \[ \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \] | 0.45 |
| Pauli-X | \[ \begin{pmatrix} 0 \\ 1 \end{pmatrix} \] | 0.00 |
| Pauli-Y | \[ \begin{pmatrix} -1 \\ 0 \end{pmatrix} \] | 0.00 |
| Pauli-Z | \[ \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \] | 0.00 |
generalized measurement operator. We will use Helstrom projective measurement in the rest of this paper for explaining our technique; however, we can also use USD for doing the same and even combine both of these techniques for different gates and faults.

For Helstrom projective measurement, we want to create an orthonormal basis \(|\omega_+\rangle\) and \(|\omega_-\rangle\) which spans \(|\psi\rangle\) and \(|\psi'\rangle\). This basis will be used for measurement and we will infer the state as \(|\psi\rangle\) or \(|\psi'\rangle\) upon measurement outcome \(|\omega_+\rangle\) or \(|\omega_-\rangle\), respectively. We want to minimize the probability of error (when state is \(|\psi\rangle\) but outcome is incorrectly \(|\omega_-\rangle\) and similarly for the other pair); so the basis states should be maximally away from the output states, i.e., \(|\langle \omega_- \vert \psi \rangle|^2 = |\langle \omega_+ \vert \psi' \rangle|^2\). We denote the corresponding probability of error by \(\delta\).

We will represent by \(ke^{ik}\) the complex number \(\langle \psi \vert \psi' \rangle = \sum_j a_j e^{-i\theta_j}\) in which \(a_j\)'s are the solution of \(OPT\) and \(e^{i\theta_j}\) are the eigenvalues of \(S = G^\dagger G_f\). We first represent our states in terms of our basis states, i.e., \(|\psi\rangle = \alpha_1 |\omega_+\rangle + \beta_1 |\omega_-\rangle\) and \(|\psi'\rangle = \alpha_2 |\omega_+\rangle + \beta_2 |\omega_-\rangle\). Without loss of generality, we can take \(\alpha_1\) as a real number \(r_1\). The condition of equal probability of error enforces these representations: \(\beta_1 = r_2 e^{i\delta x_1}\) for some real \(r_2 = \sqrt{1-r_1^2}\), \(\alpha_2 = r_2 e^{i\delta x_2}\) and \(\beta_2 = r_2 e^{i\delta x_3}\). The inner product \(|\langle \psi \vert \psi' \rangle|\) then simplifies to \(r_1 r_2 e^{-i\delta (1+e^{ix_2-x_3})}\) which we need to equate to \(ke^{ik}\). One possible solution is given by: \(x_1 = 0\), \(x_2 = -\kappa\), \(x_3 = \kappa\) and \(r_{1,2} = (\sqrt{1+k} \pm \sqrt{1-k})/2\) which produces this basis.

\[
\begin{align*}
|\omega_+\rangle &= \frac{r_1}{r_1^2 - r_2^2 e^{-2i\kappa}} |\psi\rangle - \frac{r_2 e^{-i\kappa}}{r_1^2 - r_2^2 e^{-2i\kappa}} |\psi'\rangle \\
|\omega_-\rangle &= \frac{-r_2 e^{-2i\kappa}}{r_1^2 - r_2^2 e^{-2i\kappa}} |\psi\rangle + \frac{r_1 e^{-i\kappa}}{r_1^2 - r_2^2 e^{-2i\kappa}} |\psi'\rangle
\end{align*}
\]

Therefore, we obtain the three following projectors to distinguish between \(|\psi\rangle\) and \(|\psi'\rangle\): \(\{P_0 = |\omega_+\rangle \langle \omega_+|, P_1 = |\omega_-\rangle \langle \omega_-|, P_2 = I - P_0 - P_1\}\) with outcomes \(0\), \(1\) and \(?\), respectively. The outcome \(0\) corresponds to the output state being \(|\psi\rangle\) and hence implies that the circuit is (probably) fault-free; similarly, outcome \(1\) implies that the \(i\)-th gate is probably faulty. Outcome \(?\) is never observed if circuit is fault-free or if the \(i\)-th gate is faulty; therefore, outcome \(?\) immediately signifies that the circuit has fault at some other gate. We capture the measurement output using triplets containing probability of different outcomes \((p(0), p(1), p(?))\). We call the combination of a \((C^0, C^i)\)-separating input and a measurement operator to distinguish between \(C^0\) and \(C^i\) as \(Test(i)\).

The probability of error after one measurement would be at most \(\delta = |\langle \psi \vert \omega_- \rangle|^2 = r_2^2 = (1/2)\sqrt{1-k^2}\) which matches the minimum probability of error in distinguishing \(|\psi\rangle\) and \(|\psi'\rangle\) by any projective measurement \(P\). This shows that \(Test(i)\) can optimally distinguish between a faulty and a fault-free \(i\)-th gate. Table 1 shows the probability of error in detecting SMGF faults for some of the commonly used quantum gates. The table demonstrates that for most gates, missing gate faults can be easily detected. If necessary, \(\delta\) could be further reduced using standard techniques of repeating a \(Test\) and reporting the majority of measurement outcomes — \(O\left(\frac{1}{\delta} \log \frac{1}{\epsilon}\right)\) repetitions are required to reduce error to \(\epsilon\).

For deciding if \(C\) is \(C^0\) or \(C^1\), we first compute the two triplets \(\mu^{ij} = (1-\delta, \delta, 0)\) for fault-free and \(\mu^{ij} = (\delta, 1-\delta, 0)\) for faulty circuit. Then we estimate the distribution of measurement outcomes by running the circuit multiple times using the separator state as input. Standard statistical techniques of classification can be used to determine if the observed distribution is obtained from \(\mu^{ij}\) or \(\mu^{ij}\). The optimum number of samples required is inversely proportional to the \(L_1\) distance of these distributions, which in our case is equal to \((1-2\delta)\). It is clear from Table 1 that just a single measurement can determine if a particular Hadamard gate is missing.

### III. DETECTING IF A CIRCUIT IS FAULTY

Having discussed our solution to the problem of deciding whether a particular gate in a quantum circuit is faulty or not, given that other gates are fault-free, now we discuss the more general case where any one gate in a circuit may be faulty. Our efficient diagnostic strategy uses a \textit{pre-processing} stage and a \textit{circuit evaluation} stage.

\textbf{Pre-processing stage:}\ The pre-processing stage takes as input a description of the circuit, along with each of the fault-free and faulty operators. First, for each gate \(G_i\), we construct the input state and measurement

![FIG. 2. Benchmark circuit 3qubit-CNOT](image-url)
operator for Test(i). Then, we construct a diagnostic table with s rows and (1 + s) columns whose (q, r)-th cell contains the triple $\pi(q, r) = (\Pr[0], \Pr[1], \Pr[?]\,)$ when Test(q) is applied to circuit $C^r$ — the probabilities can be obtained by using any quantum circuit simulator, such as QuIDDPro\textsuperscript{13}. Diagnostic tables for a benchmark circuit 3qubitcnot (illustrated in Figure 2) are given in the Table \textbf{II}.

\begin{table*}[h]
\begin{tabular}{|l|c|c|c|c|c|c|}
\hline
Test & $C^0$ & $C^1$ & $C^2$ & $C^3$ & $C^4$ & $C^5$ \\
\hline
Test(F1) & (1.00,0.00,0.00) & (0.00,1.00,0.00) & (0.00,0.56,0.44) & (0.07,0.50,0.43) & (0.94,0.01,0.05) & (0.98,0.01,0.01) & (0.38,0.13,0.49) \\
Test(F2) & (1.00,0.00,0.00) & (0.75,0.12,0.15) & (0.00,1.00,0.00) & (0.50,0.00,0.50) & (0.87,0.00,0.13) & (0.99,0.00,0.01) & (0.76,0.00,0.24) \\
Test(F3) & (1.00,0.00,0.00) & (0.00,1.00,0.00) & (0.50,0.00,0.50) & (0.00,1.00,0.00) & (0.87,0.06,0.07) & (0.98,0.00,0.02) & (0.86,0.00,0.14) \\
Test(F4) & (0.75,0.25,0.00) & (0.75,0.25,0.00) & (0.37,0.13,0.50) & (0.00,0.00,1.00) & (0.25,0.75,0.00) & (0.74,0.25,0.01) & (0.19,0.07,0.74) \\
Test(F5) & (0.60,0.40,0.00) & (0.40,0.27,0.33) & (0.20,0.30,0.50) & (0.55,0.38,0.07) & (0.52,0.35,0.13) & (0.40,0.60,0.00) & (0.25,0.25,0.50) \\
Test(F6) & (1.00,0.00,0.00) & (0.56,0.08,0.36) & (0.06,0.22,0.72) & (0.10,0.42,0.48) & (0.87,0.02,0.11) & (0.99,0.01,0.00) & (0.00,1.00,0.00) \\
\hline
\end{tabular}
\caption{Diagnostic fault table for circuit 3qubitcnot with single missing gate faults using Helstrom projective measurements}
\end{table*}

\textbf{Circuit evaluation stage:} During circuit evaluation stage, we get an input circuit $C$ on which we can apply any Test from \{$Test(F1) \ldots Test(Fs)\}$. Suppose we apply $Test(Fi)$ (for some chosen $i$) enough number of times to create an output distribution $\hat{\pi}$. If $C = C^i$, then $\hat{\pi}$ will be “closest” to the distribution $\pi(i, j)$. What is required is therefore an efficient way to classify $C$ into the classes \{$C^0 \ldots C^s\}$ by multiple applications of suitable Tests. It is clear that $Test(j)$ will be able to identify between $C^0$ and $C^1$ since the L1 distance of $\pi(j, 0)$ and $\pi(j, 1)$ is at least $(1 - 2\delta)$ ($\delta$ is a property of the $j$-th gate as explained earlier). However, in practice it is possible that a particular $Test(i)$ is able to distinguish between more than two classes of faults. The diagnostic table for the 3qubitcnot circuit shows that most Tests are able to easily classify all $C^i$, except $C^5$ & $C^0$ in some cases. Therefore, $Test(1)$ followed by $Test(5)$, a few applications of each, suffices to diagnose all faults – less that 20 evaluations of $C$ which is a huge improvement compared to earlier works \cite{2,3}.

\section{IV. CONCLUSION}

In this letter we present a clear outline on how one should diagnose faults in quantum circuits in the framework of ATPG. Our explanation is mostly based on single gate faults, but the techniques can be extended to certain types of multiple faults, though the computational costs would naturally increase in such cases. We show how to isolate every type of fault using very few test patterns compared to existing techniques. Our main contribution here is to demonstrate that while studying faults in quantum circuits, one should consider the properties of quantum circuits for choosing proper quantum input states as well as proper strategy of measurement for efficient testing of circuits.

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