Quantum circuit synthesis for generalized coherent states

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We present a method that outputs a sequence of simple unitary operations to prepare a given quantum state that is a generalized coherent state. Our method takes as inputs the expectation values of some relevant observables on the state to be prepared. Such expectation values can be estimated by performing projective measurements on $O(M^2 \log(M/\delta)/\epsilon^2)$ copies of the state, where $M$ is the dimension of an associated Lie algebra, $\epsilon$ is a precision parameter, and $1-\delta$ is the required confidence level. The method can be implemented on a classical computer and runs in time $O(M^6 \log(M/\epsilon))$. It provides $O(M \log(M/\epsilon))$ simple unitaries that form the sequence. The number of all computational resources is then polynomial in $M$, making the whole procedure very efficient in those cases where $M$ is significantly smaller than the Hilbert space dimension. When the algebra of relevant observables is determined by some Pauli matrices, each simple unitary may be easily decomposed into two-qubit gates. We discuss applications to quantum state tomography and classical simulations of quantum circuits.

I. INTRODUCTION

An important problem in quantum information theory regards the determination of a pure multiparty quantum state $|\psi\rangle$. This problem has many applications, including quantum device and quantum state verification. The most general procedure to determine $|\psi\rangle$ is via quantum state tomography [1]. In this case, a complete set of observables must be measured on multiple copies of the state. The number of measurements depends then on the number of observables as well as the precision and confidence levels required in the state reconstruction. This number is prohibitively large in general, i.e., it is polynomial in the Hilbert space dimension or exponential in the size of the quantum system [2].

For this reason, some recent approaches focus on cases where a form of quantum state tomography can be performed efficiently (c.f., [3][4]). These approaches work only for particular classes of states and do not apply generally. Also of interest are quantum tomographic approaches for more general pure quantum states that can be prepared by a quantum computer via a quantum circuit. This problem may be important for the validation and verification of quantum computing devices, which is also studied in Refs. [5][6] from a different viewpoint. In this problem, the assumption is that the length of the quantum circuit is significantly (exponentially) smaller than the Hilbert space dimension. Then, an efficient description for the prepared quantum state $|\psi\rangle$ is given by the unitary operators that form the circuit. That is, quantum state tomography of $|\psi\rangle$ is also achieved by providing a quantum circuit that prepares it. As in general quantum state tomography, the quantum circuit may be obtained by measuring certain observables on multiple copies of $|\psi\rangle$. Once the quantum circuit is known, additional information about the state may be obtained efficiently using classical resources.

Some known results already use this “quantum circuit” approach to quantum state tomography. In Ref. [3], for example, an efficient method for quantum state tomography of matrix product states is given. It is shown that, by obtaining the reduced density matrices of the $n$-qubit quantum state $|\psi\rangle$, a quantum circuit of size polynomial in $n$ that prepares $|\psi\rangle$ can be constructed. In Ref. [4], a similar approach is analyzed for the so-called stabilizer states. That approach is based on performing Bell measurements to determine a complete set of generators for the stabilizer operators. Using the results of Ref. [4], a quantum circuit of polynomial size that prepares the stabilizer state can be obtained. We note that in these examples, knowing a quantum circuit that prepares the state also allows for the efficient classical computation of expectation values of other observables on $|\psi\rangle$.

Here, we analyze this approach in the case of generalized coherent states (GCSs). We call our approach quantum circuit synthesis for GCSs as the problem reduces to finding a sequence of simple unitary transformations that prepare a given GCS, when acting on some trivial initial state. When dealing with $n$-qubit systems, each unitary transformation may be easily decomposed into a polynomially large sequence of two-qubit gates, in the worst case, and the initial state may be $|00\ldots0\rangle$. When dealing with quantum systems obeying different particle statistics, such as fermionic or bosonic systems, the results in Refs. [7][8] may be useful for simulating such systems on quantum computers and devising quantum circuits that implement the unitary transformations.

GCSs have the nice property that are uniquely determined by the expectation values of certain observables. These observables form a basis of an associated Lie algebra. For many important cases, the number of observables in the basis is significantly (exponentially) smaller than the Hilbert space dimension. It is then reasonable to consider and develop efficient methods that take the expectation values as input and provide the sequence of unitary transformations that prepare the GCS as output. We provide one such method in this paper.

Our main result can be interpreted as an efficient quantum-circuit approach to quantum state tomography of GCSs. The number of copies of the state needed to
estimate the expectation values of observables and the number of classical operations to find the unitaries (or quantum circuit) scales polynomially with \( M, 1/\epsilon, \) and \( \log(1-\delta) \). Here, \( M \) is the dimension of the associated Lie algebra, \( \epsilon > 0 \) is a precision parameter, and \( \delta < 1 \) is the confidence level. The latter appears naturally from the estimation of the expectation values by repeated measurements. Our method relies heavily on a diagonalization procedure that is suitable for Lie algebras \(^{11, 12}\), and which is a generalization of the Jacobi method to diagonalize matrices.

Additional implications of our main result are in order. First, the results in Ref. \(^{13}\) can be used to obtain estimates of certain unitary operations and other observables on the GCS efficiently, using only classical resources. Such observables do not necessarily belong to the Lie algebra. Second, our techniques can be applied to simulate certain classes of quantum circuits efficiently on a classical computer.

Our paper is organized as follows. In Sec. \(^{11}\) we introduce GCSs and give some results about semisimple Lie algebras. In Sec. \(^{111}\) we formalize the problem that we are solving. In Sec. \(^{1111}\) we provide the details of our method, describe the diagonalization procedure, and obtain bounds for the number of copies of the state and classical operations required. In Sec. \(^{11111}\) we discuss further applications of our results to the efficient classical simulation of certain quantum circuits.

II. GENERALIZED COHERENT STATES

To introduce GCSs \(^{11, 16}\), we focus on the case where a set of observables (Hermitian operators) form a semisimple Lie algebra \( \mathfrak{h} \) of linear operators acting on a finite dimensional Hilbert space \( \mathcal{H} \). The Hilbert space can be that of a multiparty quantum system. We assume \( \mathfrak{h} \) to be a real Lie algebra of dimension \( M \). The bracket of two observables \( O_x \) and \( O_y \) is given by \( [O_x, O_y] = i(O_x O_y - O_y O_x) \), which is familiar to physicists. We also assume that \( \mathfrak{h} \) acts irreducibly on \( \mathcal{H} \).

If \( O_x \in \mathfrak{h} \), the Lie group generated by \( \mathfrak{h} \) involves the map \( O_x \to e^{iO_x} \). GCSs associated with \( \mathfrak{h} \) are the pure quantum states

\[
\{ |\psi\rangle \equiv e^{i\mathfrak{h}} |\text{hw}\rangle \},
\]

where \( e^{i\mathfrak{h}} \) is any unitary Lie group operation, commonly referred to as a displacement operator. \( |\text{hw}\rangle \) is a pure quantum state that represents the highest-weight state of \( \mathfrak{h} \), as explained below. That is, GCSs belong to the unique orbit of a highest-weight state of \( \mathfrak{h} \) under the action of the Lie group.

As \( \mathfrak{h} \) is semisimple, it assumes a Cartan-Weyl basis decomposition: \( \mathfrak{h}_D \oplus \mathfrak{h}^{+} \oplus \mathfrak{h}^{-} \). The subalgebra \( \mathfrak{h}_D \) is the Cartan subalgebra (CSA) and is spanned by the largest set of commuting observables in \( \mathfrak{h} \). The generators of the CSA are \( H_1, \ldots, H_R \). \( \mathfrak{h}^{+} \) is spanned by \( L \) raising operators \( E_1^+, \ldots, E_L^+ \) and \( \mathfrak{h}^{-} \) is spanned by \( \mathfrak{L} \) lowering operators \( E_1^-, \ldots, E_L^- \). The weight states of \( \mathfrak{h} \) are simultaneously eigenstates of all observables in \( \mathfrak{h}_D \). In particular, given a Cartan-Weyl basis for \( \mathfrak{h} \), the highest-weight state \( |\text{hw}\rangle \) is a weight state that satisfies

\[
E_l^+ |\text{hw}\rangle = 0, \quad \forall 1 \leq l \leq L.
\]

The weights of \( |\text{hw}\rangle \), \( w : \mathfrak{h}_D \to \mathbb{R} \), are defined by \( H_i |\text{hw}\rangle = w(H_i) |\text{hw}\rangle \).

The GCSs given by Eq. \(^{1}\) should be compared with the well-known Glauber coherent states appearing in quantum optics \(^{20}\). That is, for coherent states, the vacuum state plays the role of the highest-weight state and the displacement operator is given by the exponential of field operators. GCSs are then a generalization of coherent states that may be suitable for finite-dimensional quantum systems.

III. STATEMENT OF THE PROBLEM

We let \( |\psi\rangle \) be a GCS associated with the Lie algebra \( \mathfrak{h} \) and \( \mathfrak{h}_D \oplus \mathfrak{h}^{+} \oplus \mathfrak{h}^{-} \) denotes a given Cartan-Weyl basis. \( |\psi\rangle \) is prepared using a black-box transformation as in Fig. \(^{1}\) and we assume that we have access to multiple copies of \( |\psi\rangle \). The goal is to obtain a sequence of simple unitary transformations \( U_1, \ldots, U_K \) such that, with probability at least \( 1-\delta \),

\[
|| |\psi\rangle - \prod_{k=1}^{K} U_k |\text{hw}\rangle || \leq \epsilon .
\]

\( \delta > 0 \) and \( \epsilon > 0 \) are given and determine the confidence level (i.e., \( 1-\delta \)) and precision of the estimation, respectively. The unitaries \( U_k \) belong to the Lie group obtained from \( \mathfrak{h} \) and, for the given Cartan-Weyl basis, they are

\[
U_k = \exp \left\{ i \left( \alpha_k E_{l(k)}^+ + \alpha_k^* E_{l(k)}^- \right) \right\},
\]

where \( \alpha_k \in \mathbb{C} \) and \( l(k) \in \{1, \ldots, L\} \).

![FIG. 1. Black-box GCS preparation. The initial state |0⟩ may represent the highest-weight state and B is a quantum operation that transforms |0⟩ into the GCS |ψ⟩.](image-url)

For qubit systems, the Lie algebra \( \mathfrak{h} \) is usually spanned by certain products of Pauli operators acting on qubit spaces. In this case, the unitaries \( U_k \) may be easily decomposed as sequences of one and two-qubit gates following, for example, the results in Ref. \(^{19}\). For some relevant Lie algebras, such as \( \mathfrak{so}(2n) \), the number of gates in this sequence scales linearly with the number of qubits, in the worst case \(^{21}\).
IV. UNITARY OPERATIONS FOR GCSs

Any GCS $|\psi\rangle$ is the unique ground state (eigenstate of lowest eigenvalue) of some observable in $\mathfrak{h}$ \cite{22}. It follows that, if $\{O_1, \ldots, O_M\}$ is a basis of observables for $\mathfrak{h}$, $|\psi\rangle$ is uniquely determined (up to an irrelevant phase factor) by the expectation values $\langle O_m \rangle_\psi = \langle \psi | O_m | \psi \rangle$, $1 \leq m \leq M$ \cite{23}. To obtain the sequence of unitaries $U_k$ of Eq. (4) that prepares a given GCS, or a quantum circuit, the first goal is then to determine the expectation values. This will require performing (projective) measurements of each $O_m$ in multiple copies of $|\psi\rangle$. The number of copies will depend on the goal precision and confidence level; however, we assume first that the expectations can be obtained exactly and analyze the effects of errors in Sec. IV.B.

Our procedure to find the $U_k$’s is as follows. From the expectation values $\langle O_m \rangle_\psi$, we will construct a Hamiltonian (i.e., an observable in $\mathfrak{h}$) that has $|\psi\rangle$ as unique eigenstate of largest eigenvalue. Then, we will invoke a classical procedure to diagonalize the Hamiltonian using Lie group operations. Such a procedure was used in Refs. \cite{11,13} in the context of generalized mean-field Hamiltonians and is based on an extension of Jacobi’s diagonalization method that applies to semisimple Lie algebras \cite{12}. The Lie group operations will correspond to the $U_k$’s. Figure 2 summarizes our approach.

![Diagram of measurement process, encoding Hamiltonian, and diagonalization procedure](image)

FIG. 2. Our approach to obtaining a sequence of unitary transformations $U_1, \ldots, U_K$ to prepare a GCS, as determined by Eq. (5).

If the basis of observables for $\mathfrak{h}$ is orthogonal, it satisfies \cite{9}:

$$\text{Tr}(O_m O_{m'}) = \mathcal{N} \delta_{mn},$$

with $\mathcal{N} > 0$. The orthogonal basis may be obtained from the given Cartan-Weyl basis, i.e.

$$
\begin{cases}
O_1 = H_1, \ldots, O_R = H_R, \\
O_{R+1} = (E_1^+ + E_1^-), \ldots, O_{R+L} = (E_L^+ + E_L^-), \\
O_{R+L+1} = i(E_1^+ - E_1^-), \ldots, O_{R+2L} = i(E_L^+ - E_L^-).
\end{cases}
$$

(A pre-processing step may be needed to satisfy Eqs. (5) and (6), but that step is not very time consuming – it may require multiplying the operators in the Cartan-Weyl basis by different constants – and will not dominate the complexity of our procedure. Then, the expectation values $\langle O_m \rangle_\psi$ are determined from the expectation values of the operators in the given Cartan-Weyl basis (and vice versa). We will assume that Eq. (6) is satisfied.

Given the relevant expectation values, we construct the following Hamiltonian in $\mathfrak{h}$:

$$F_\psi = \sum_{m=1}^{M} O_m \langle O_m \rangle_\psi.$$  

For any pure quantum state $|\phi\rangle \in \mathcal{H}$, it is known that

$$0 \leq \sum_{m=1}^{M} (O_m)_{\phi}^2 \leq P_\phi,$$

where $P_\phi > 0$ is the so-called purity relative to the algebra $\mathfrak{h}$ (or $\mathfrak{h}$-purity). Furthermore, for any GCS $|\psi\rangle$ associated with $\mathfrak{h}$, we have

$$\sum_{m=1}^{M} (O_m)_{\psi}^2 = P_\psi.$$

The $\mathfrak{h}$-purity is then invariant under Lie group transformations. Quantum states that are not GCSs have $\mathfrak{h}$-purity strictly less than $P_\phi$—see Ref. \cite{22} for more details.

The Cauchy-Schwarz inequality implies

$$|\langle F_\psi \rangle_\phi| \leq \left| \sum_{m=1}^{M} (O_m)_{\phi} \langle O_m \rangle_\psi \right| \leq P_\psi.$$

Furthermore, the upper bound is tight and is only obtained when $|\phi\rangle = |\psi\rangle$, since $\langle F_\psi \rangle_\phi$ reduces to the $\mathfrak{h}$-purity defined in Eq. (4). As GCSs are uniquely determined by the expectation values of the basis operators, the state $|\psi\rangle$ is then the unique eigenstate of $F_\psi$ of largest eigenvalue $P_\psi$.

We let $U$ be the Lie group operation that transforms $|\text{hw}\rangle$ into the GCS $|\psi\rangle$ as in Eq. (1). We also define the Hamiltonian $F_{\text{hw}} = \sum_{r=1}^{R} w(H_r)H_r$, where $w(H_r) \in \mathbb{R}$ are the eigenvalues of $|\text{hw}\rangle$ associated with each $H_r$ (weights). In the following, we will show $U^\dagger F_{\psi} U = F_{\text{hw}}$. That is, $U$ can be used to diagonalize $F_\psi$. By diagonalization we mean a particular transformation that takes an element of $\mathfrak{h}$ and maps it into an observable in $\mathfrak{h}_D$.

From Eq. (2), the raising and lowering operators satisfy $(E_l^\pm)_{\text{hw}} = 0$ for all $l$. Then, Eq. (6) implies $F_{\text{hw}} = \sum_{m=1}^{M} (O_m)_{\psi} O_m$. The unique eigenstate of $F_{\text{hw}}$ of largest eigenvalue $P_\psi$ is then $|\text{hw}\rangle$. Since $U$ is a unitary transformation in the Lie group, we obtain

$$U F_{\text{hw}} U^\dagger = \sum_{m=1}^{M} c_m O_m,$$

where $c_m \in \mathbb{R}$. We can obtain the coefficients using Eq. (5) as follows:

$$c_m = \text{Tr}(U F_{\text{hw}} U^\dagger O_m) / \mathcal{N}.$$  

(12)

With no loss of generality, $U^\dagger O_m U = \sum_{m'=1}^{M} d_{mm'} O_{m'}$, where $d_{mm'} \in \mathbb{R}$. Then, Eq. (12) can be rewritten as

$$c_m = \sum_{r=1}^{R} d_{mr} w(H_r).$$  

(13)
Similarly,
\[
\langle \text{hw} | U^\dagger O_m U | \text{hw} \rangle = \sum_{m'=1}^{M} d_{mm'} \langle \text{hw} | O_{m'} | \text{hw} \rangle = \sum_{r=1}^{R} d_{mm} w(H_r). \tag{14}
\]
As Eqs. (13) and (14) coincide, we obtain \( c_m = \langle O_m \rangle \) and
\[
F_{\text{hw}} = U^\dagger F_{\psi} U. \tag{15}
\]

We now assume there exists a classical procedure to diagonalize \( F_\psi \) that outputs a sequence of Lie-group unitaries \( V_1, V_2, \ldots \), that form a unitary \( V \). We also let each \( V_k \) be an exponential like the one in Eq. (4). By the assumption, \( V^\dagger F_\psi V \) is an element of the CSA; we define it as \( F_D \). The largest eigenvalue of \( F_D \) is also \( D \) and the corresponding eigenvector is the weight state \(|w\rangle\).

In principle, \( F_D \neq F_{\text{hw}} \). The equality would only hold if \(|w\rangle = |\text{hw}\rangle\). Nevertheless, since both \( V \) and \( U \) are in the Lie group, there is a Lie group transformation that takes \(|w\rangle \rightarrow |\text{hw}\rangle\) and thus \( F_D \rightarrow F_{\text{hw}} \). This last transformation can be built upon a sequence of Weyl-group reflections. The sequence can be determined efficiently in \( M \) and each reflection also takes the form of Eq. (4) – see Thm. 2.63 in Ref. [24].

A. Diagonalization procedure

A sequence of unitaries having the form of Eq. (4) can then be obtained via a classical procedure that diagonalizes \( F_\psi \). This procedure is discussed in Sec. 5.2.1 of Ref. [11] and is based on Ref. [12]. It can be interpreted as a generalization of Jacobi’s diagonalization method suitable to the case of Lie algebras. While in this section we analyze the steps to diagonalize \( F_\psi \), the same procedure can be used to diagonalize any Hamiltonian in \( \mathfrak{h} \). We summarize the procedure here for completeness, while still providing more details than Ref. [11]. The actual complexity of this procedure for our problem is determined in Sec. [IV B].

As before, we assume that the expectations \( \langle O_m \rangle \) are exactly known and analyze the effects of errors in these expectations in Sec. [IV B]. To be exact, the diagonalization procedure should involve infinitely many steps. Nevertheless, the number of steps can be made finite with controlled errors. We define a sequence of Hamiltonians in \( \mathfrak{h} \), \( \{F_0^{(0)}, F_1^{(1)}, \ldots\} \), with \( F_0^{(0)} = F_\psi \). Step \( k \) takes \( F_\psi^{(k-1)} \) as input and outputs \( F_\psi^{(k)} \), which is closer to being diagonal, according to a measure that provides the distance between observables in \( \mathfrak{h} \) and the CSA – see Sec. [IV B]. From Eq. (6), each \( F_\psi^{(k)} \) admits the following representation:
\[
F_\psi^{(k)} = \sum_{r=1}^{R} \gamma_r^k H_r + \sum_{l=1}^{L} (\xi^l E_l^{(k)} + (\xi^l)^* E_l^{(k)}) \tag{16}
\]
The coefficients \( \gamma^k_r \) and \( \xi^k_l \) may be obtained from the initial expectation values \( \langle O_m \rangle \). We need to update and store in memory the coefficients \( \gamma^k_r \) and \( \xi^k_l \) at each step.

Before describing each step, we present some results from the theory of semisimple Lie algebras that will be useful. For each \( l \), the operators \( E_l^+, E_l^- \), and some observable in the CSA form an \( \mathfrak{su}(2) \) algebra (Thm. 7.19 of [19]). This algebra can be obtained as follows. First, we compute the commutator \( [E_l^+, E_l^-] = Z_l \), where \( Z_l \) is nonzero and \( Z_l \in \mathfrak{h}^\perp \); we write \( Z_l = \sum_{r=1}^{R} \mu_r H_r \). Then, we compute \( [E_l^+, Z_l] = \eta_l Z_l \); with no loss of generality, \( \eta_l > 0 \) (otherwise replace \( E_l^+ \) by \( E_l^- \)). The \( \mathfrak{su}(2) \) algebra is constructed from \( S_l^+ = E_l^+ / \sqrt{\mu_l}, S_l^- = E_l^- / \sqrt{\mu_l}, \) and \( S_l^z = Z_l / \eta_l \). These operators satisfy the usual \( \mathfrak{su}(2) \) commutation relations: \( [S_l^+, S_l^-] = S_l^z \) and \( [S_l^x, S_l^y] = \pm S_l^z \). Alternatively, we can define the observables \( S_l^z = (S_l^+ + S_l^-) / \sqrt{2} \) and \( S_l^y = i(S_l^+ - S_l^-) / \sqrt{2} \). In physics, these observables are associated with the angular momentum operators.

At the \( k \)-th step of the diagonalization procedure, we search for the value of \( \lambda^k_l \) such that \( |\gamma^k_l| > |\eta^l_k|^k \), for all \( l \in \{1, \ldots, L\} \). We then construct a unitary \( V_k \) that is of the form \( e^{i(\alpha_k E_l^0 + \alpha_k^* E_l^0)} \). This unitary will be used to transform \( F_\psi^{(k-1)} \) into \( F_\psi^{(k)} \). The coefficients \( \alpha_k \) can be obtained as follows. With no loss of generality,
\[
F_\psi^{(k-1)} = S_l^+ X_l^+ + \xi^x S_l^x + \xi^y S_l^y + X_l^+, \tag{17}
\]
where \( \xi^x, \xi^y, \xi^z \in \mathbb{R} \) and \( X_l^+ \in \mathfrak{h} \) is a Hamiltonian that is orthogonal to the corresponding \( \mathfrak{su}(2) \) algebra, according to the inner product of Eq. (6). The constants satisfy
\[
\xi^x = \eta_l \sum_{r=1}^{R} \gamma_r^{(k-1)} \mu_r, \tag{18}
\]
\[
\xi^y = i \eta_l \sum_{r=1}^{R} \gamma_r^{(k-1)} \mu_r, \tag{19}
\]
and
\[
\xi^z = - \sum_{r=1}^{R} (\mu_r)^2. \tag{20}
\]
The coefficients \( \eta_l \) and \( \mu_r \) are previously known, and the coefficients \( \gamma_r^{(k-1)} \) are also known from the \((k-1)\)-th step. Further details about Eq. (20) are discussed in Appendix [A]. The unitary operation \( V_k \) is the one that diagonalizes the Hamiltonian \( \xi^x S_l^x + \xi^y S_l^y + \xi^z S_l^z \), which appears on the right hand side of Eq. (17), and transforms it to an observable that is proportional to \( S_l^z \). Thus, \( V_k \) is \( e^{i(\pi^x S_l^x + \pi^y S_l^y)} \), where the coefficients are
\[
\pi^x = \theta \xi^y, \pi^y = - \theta \xi^x, \tag{21}
\]
and the rotation angle or phase is
\[
\theta = \arctan \left( \frac{\sqrt{\xi^x^2 + \xi^y^2}}{\xi^x} \right). \tag{22}
\]
The described diagonalization procedure is guaranteed to output a diagonal Hamiltonian only when the number of steps, \( K' \), is infinity. For \( K' < \infty \), the resulting Hamiltonian is only almost diagonal, in the following sense. We let \( d^k = \sum_{l=1}^{L} |\lambda_l^k|^2 \) be the (squared) distance of \( F^k_{\psi} \) to the CSA. In particular, \( d^k = 0 \) if and only if \( F^k_{\psi} \) is diagonal, i.e., it belongs to the CSA. Equation 5.63 of Ref. 11 implies that

\[
K' \geq \frac{\log(d^0/\epsilon_D)}{\log((L + 1)/L)}
\]

steps of the diagonalization procedure suffice to achieve \( d^{K'} \leq \epsilon_D \). That is, \( K' = O(L \log(d^0/\epsilon_D)) \), assuming \( d^0 \geq \epsilon_D \). Additionally, the expectation values \( \langle O_m \rangle_\psi \) can only be estimated within certain precision and confidence levels by finitely-many measurements. It follows that we can only provide a sequence of simple unitaries to prepare a quantum state that is \( \epsilon \)-close to the GCS and with confidence level \( 1 - \delta \) — see Sec. 11. For given \( \epsilon \) and \( \delta \), the complexity of the diagonalization procedure and the
number of measurements can be determined, as shown below.

The actual input Hamiltonian to the diagonalization procedure is

$$\tilde{F}_\psi = \sum_{m=1}^M O_m \langle \tilde{O}_m \rangle_\psi .$$

(26)

Here, $\langle \tilde{O}_m \rangle_\psi$ are the estimates of the expectations, and we assume that each estimate is obtained within precision $\epsilon_M$. The Hamiltonian obtained at the $k$-th step is $\tilde{F}_\psi^k = (\tilde{V}_k)^\dagger \tilde{F}_\psi^{k-1} \tilde{V}_k$, where $\tilde{V}_k$ is the Lie-group transformation discussed in Sec. [IV A] After $K'$ steps, the Hamiltonian is $\tilde{F}_\psi^{K'}$, and this may not be in the CSA. To this end, we regard as the output of the procedure the projection of $\tilde{F}_\psi^{K'}$ into the CSA, that is, its diagonal part. We define it to be $\tilde{F}_\psi^{CSA}$.

It is useful to define $\| O \| = \max_{1 \leq m \leq M} \| O_m \|$ as the maximum of the operator norm of the observables in the orthogonal basis of $\mathcal{h}$. We first set $\epsilon_D$ and $K'$. Under the assumption that $\epsilon_M \ll 1$, the eigenvalues of $\tilde{F}_\psi$ are sufficiently close to those of $F_\psi$. That is, the largest eigenvalue of $\tilde{F}_\psi$ is close to $P_0$ and the second largest one is close to $P_\mathcal{h} - \Delta$, where $\Delta > 0$ is the spectral gap of $F_\psi$. We will set a lower bound on $\Delta$ below. In Appendix [B] we use perturbation theory to show that there is $\epsilon_D = \Omega(\epsilon^2 \Delta^2/(L\| O \|^2))$ such that $\tilde{F}_\psi^{K'}$ is sufficiently close to being diagonal. That is, if $|\tilde{w}_0\rangle$ is the eigenstate of largest eigenvalue of $\tilde{F}_\psi^{CSA}$ and $\tilde{V}^l$ is the unitary transformation to obtain $\tilde{F}_\psi^{K'}$ from $\tilde{F}_\psi$, then

$$\| \psi \rangle - \tilde{V} |\tilde{w}_0\rangle\| = \mathcal{O}(\epsilon) ,$$

(27)

in the limit $\epsilon_M \to 0$. According to Eq. (25), the number of steps is

$$K' = \mathcal{O} \left( L \log \left( \frac{d^0 L \| O \|^2}{\epsilon^2 \Delta^2} \right) \right) .$$

(28)

A sequence of Weyl reflections can transform $|\tilde{w}_0\rangle$ into $|\mathsf{hw}\rangle$ as

$$U_{K'+1} \ldots U_K |\mathsf{hw}\rangle = |\tilde{w}_0\rangle .$$

(29)

In Appendix [B] we also show that it suffices to have estimates of the expectations within precision $\epsilon_M = \Omega(\epsilon \Delta/\| O \|)$. (We assume, for simplicity, that all estimates are obtained within the same precision.) This choice of $\epsilon_M$ also implies Eq. (27).

If we perform projective measurements of each $O_m$ on $|\psi\rangle$, we obtain values $O_m$ with probabilities $p_m$. According to Hoeffding’s inequality [25], after performing $Q$ projective measurements of $O_m$ to get the estimate $\langle \tilde{O}_m \rangle_\psi$, we obtain

$$\Pr \left( \| \langle \tilde{O}_m \rangle_\psi - \langle O_m \rangle_\psi \| \geq \epsilon_M \right) \leq 2e^{-\frac{Q \epsilon_M^2}{2d^0 L \| O \|^2}} .$$

(30)

We use a union bound for which, if the overall desired confidence level is $1 - \delta$, the confidence level in the estimation of each expectation value is, at least, $1 - \delta/M$. Under this assumption, it suffices to have a number of measurements for each $O_m$ that satisfies

$$Q = \left| \frac{2\| O \|^2 \log(2M/\delta)}{\epsilon_M^2 \mathcal{O}} \right| .$$

(31)

The total number of measurements for all observables is $QM$.

Since $L = \mathcal{O}(M), d^0 = \mathcal{O}(M\| O \|)$, and $\epsilon_D = \Omega(\epsilon^2 \Delta^2/(M\| O \|^2))$, Eq. (28) is

$$K' = \mathcal{O} \left( M \log \left( \frac{M^2 \| O \|^4}{\epsilon^2 \Delta^2} \right) \right) .$$

(32)

The number of steps $K'$, in addition to the $\mathcal{O}(M)$ Weyl reflections of Eq. (29), is the total number of unitaries $K$ of Eq. (30). The complexity of the diagonalization procedure, as discussed in Sec. [IV A], is $\mathcal{O}(K'M^3)$. This is

$$\mathcal{O} \left( M^4 \log \left( \frac{M^2 \| O \|^4}{\epsilon^2 \Delta^2} \right) \right) ,$$

(33)

and thus polynomial in the dimension of $\mathcal{h}$. The number of projective measurements is

$$Q,M = \mathcal{O} \left( \frac{M^3 \| O \|^4 \log(M/\delta)}{\epsilon^2 \Delta^2} \right) ,$$

(34)

which was obtained using Eq. (31) and $\epsilon_M = \Omega(\epsilon \Delta/\| O \|)$. This number is also polynomial in $M$.

Last, we make a remark about the spectral gap $\Delta$, which is also the spectral gap of $F_{\mathsf{hw}}$. By construction, $\Delta$ scales as $\| O \|^2$ in the sense that $\Delta \to \kappa^2 \Delta$ if we replace $O_m \to \kappa O_m$, $\kappa > 0$. $\Delta$ can be determined from the commutation relations of $\mathcal{h}$ or, more precisely, by the structure constants of the algebra. This is because other weight states can be obtained from $|\mathsf{hw}\rangle$ by acting with the lowering operators, and the structure constants can be used to determine the weights and eigenvalues of the observables in the CSA. As these structure constants are, a priori, independent of the dimension $M$, the second largest eigenvalue of $F_{\mathsf{hw}}$ has to be at a gap of order $c\| O \|^2$ from the largest eigenvalue, with $c = \mathcal{O}(1)$.

Then, the complexity of the diagonalization procedure is $\mathcal{O}(M^4 \log(M/\epsilon))$ and the number of projective measurements is $\mathcal{O}(M^4 \log(M/\delta)/\epsilon^2)$. The unitaries of Eq. (29) together with the $K'$ unitaries $U_k := \tilde{V}_k$, which result from the diagonalization procedure applied to $F_\psi$, provide the $K$ unitaries that satisfy Eq. (30).

V. APPLICATIONS TO THE SIMULATION OF QUANTUM CIRCUITS

In Ref. [13] we introduced the model of Lie-algebraic quantum computing (LQC). In this model, the set of
gates is induced by the control Hamiltonians that belong to a semisimple Lie algebra \( \mathfrak{h} \), and that set may not be universal. The initial state is a ground state of a control Hamiltonian (e.g., a highest-weight state) and the final measurement is an expectation of either a control Hamiltonian or a unitary operator in the group generated by \( \mathfrak{h} \). Thus, the expectation values after the action of \( \mathfrak{h} \) can be obtained from the previous ones in time that is polynomial in \( M \), under the assumptions. In particular, we can compute the expectation values \( \langle O_m \rangle_{\psi_\mathcal{L}} \) of the final state on a classical computer in time that is polynomial in \( M \) and linear in the length of the quantum circuit, \( \mathcal{L} \).

If the goal is to obtain an expectation value of an observable in \( \mathfrak{h} \) on \( |\psi_\mathcal{L}\rangle \), such an expectation can be readily obtained from the computed \( \langle O_m \rangle_{\psi_\mathcal{L}} \)’s. If, however, the goal is to obtain the expectation value of a unitary operator in the group or an observable that is not in \( \mathfrak{h} \), we can proceed as follows. First, from the \( \langle O_m \rangle_{\psi_\mathcal{L}} \)’s we build the Hamiltonian

\[
F_{\psi_\mathcal{L}} = \sum_{m=1}^{M} O_m \langle O_m \rangle_{\psi_\mathcal{L}}.
\]

Then, we run the diagonalization procedure described in Sec. [IV.A] to obtain a sequence of Lie-group operations that prepare \( |\psi_i\rangle \) from the highest-weight state. Once such a sequence is obtained, we have reduced the problem to that of simulating LQC, which can be done efficiently using classical resources according to the results in Ref. [13].

Note that, for precision \( \epsilon \) in the computation of the expectation value, the number of Lie-group unitaries obtained by the diagonalization procedure is \( \mathcal{O}(M \log(M/\epsilon)) \). The complexity for implementing the diagonalization procedure is \( \mathcal{O}(M^4 \log(M/\epsilon)) \). Then, the overall complexity for classically simulating the quantum computation in this case is efficient; that is, polynomial in \( M \) and linear in \( \mathcal{L} \).

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Appendix A: Coefficients for $su(2)$ operations

As pointed out in Eqs. (10) and (17), we can write

$$ F_{k-1}^{\psi} = \sum_{r=1}^{R} \xi_r^{k-1} H_r + \ldots $$

(A1)

$$ = \xi^{k} S_{0}^{\psi} + \ldots , $$

(A2)

where the coefficients $\xi_{r}^{k-1}$ are stored in memory. The remaining terms in the right hand side of Eq. (A1) are in $\mathfrak{h}^+ \oplus \mathfrak{h}^-$. The remaining terms in the right hand side of Eq. (A2) are linear combinations of $S_{r}^{\psi}$ and $S_{0}^{\psi}$, and other observables orthogonal to the corresponding $su(2)$ algebra.

We seek to find the coefficient $\xi^{k}$ of Eq. (A2). Using Eq. (5) and $Z_{l'} = \sum_{r=1}^{R} \mu_{r} H_{r}$, on one hand we have

$$ \text{Tr}[F_{k-1}^{\psi} Z_{l'}] = N \sum_{r=1}^{R} \xi_{r}^{k-1} \mu_{r} . $$

(A3)

On the other hand, since $S_{0}^{\psi} = Z_{l'}/\eta_{l'}$, we have

$$ \text{Tr}[F_{k-1}^{\psi} Z_{l'}] = (\xi^{k/\eta_{l'}}) \text{Tr}[(Z_{l'})^{2}] $$

(A4)

$$ = N (\xi^{2/\eta_{l'}}) \sum_{r=1}^{R} (\mu_{r})^{2} . $$

Then,

$$ \xi^{k} = \frac{\eta_{l'} \sum_{r=1}^{R} \xi_{r}^{k-1} \mu_{r}}{\sum_{r=1}^{R} (\mu_{r})^{2}} , $$

(A5)

which coincides with Eq. (20).

Appendix B: Approximation errors and perturbation theory

Given a Cartan-Weyl basis, the observables that determine an orthogonal basis for $\mathfrak{h}$ are given by Eq. (9). Then, $\| E_{l}^{\perp} \| \leq \| O \|$ for all $l \in \{ 1, \ldots, L \}$. When the input to the diagonalization procedure is $F_{\psi}$, the coefficients of the output Hamiltonian, after $K'$ steps, satisfy $\sum_{l=1}^{L} | h_{l}^{K'} |^{2} \leq \epsilon_{D}$. Also, the term of $F_{\psi}^{K'}$ that does not belong to the CSA has an operator norm that is upper bounded by

$$ 2 \| O \| \sum_{l=1}^{L} | h_{l}^{K'} | \leq 2 \| O \| \sqrt{\epsilon_{D} L} , $$

(B1)

where the last inequality follows from a property between the 1- and 2-norm of complex vectors.

The Hamiltonian $F_{\psi}^{K'}$ can be written as

$$ F_{\psi}^{K'} = F_{\psi}^{\text{CSA}} + F_{\psi}^{\perp} , $$

(B2)

where $F_{\psi}^{\text{CSA}} \in \mathfrak{h}^{+}$ and $F_{\psi}^{\perp}$ is orthogonal to the CSA in the sense of Eq. (5): that is $F_{\psi}^{\perp} \in \mathfrak{h}^{+} \oplus \mathfrak{h}^{-}$. Equation (B1) implies

$$ \| F_{\psi}^{\perp} \| = O \left( \| O \| \sqrt{\epsilon_{D} L} \right) . $$

(B3)

We let $| w_{0} \rangle$ be the eigenstate (weight state) of largest eigenvalue of $F_{\psi}^{\text{CSA}}$ and $| w_{1} \rangle$ be the eigenstate of largest eigenvalue of $F_{\psi}^{K'}$. Note that $| w_{1} \rangle$ is not, in principle, a weight state. We seek an expression for an upper bound on $\| | w_{1} \rangle - | w_{0} \rangle \|$, which can be obtained from perturbation theory. $\epsilon_{D}$ will then be obtained by requiring such a bound to be $O(\epsilon)$.

To obtain this bound, we parametrize the Hamiltonian as

$$ F_{\psi}^{K'}(s) = F_{\psi}^{\text{CSA}} + s F_{\psi}^{\perp} , $$

(B4)

with $0 \leq s \leq 1$. The eigenstate of largest eigenvalue is defined to be $| w_{s} \rangle$. In the perturbative regime, where the dominant term in the Hamiltonian is $F_{\psi}^{\text{CSA}}$, $| w_{s} \rangle$ determines a differentiable path in Hilbert space. Then,

$$ \| | w_{1} \rangle - | w_{0} \rangle \| = \left\| \int_{0}^{1} ds \partial_{s} | w_{s} \rangle \right\| $$

$$ \leq \int_{0}^{1} ds \| \partial_{s} | w_{s} \rangle \| $$

$$ \leq \max_{0 \leq s \leq 1} \| \partial_{s} | w_{s} \rangle \| . $$

(B5)

We can use the eigenvalue equation $F_{\psi}^{K'}(s) | w_{s} \rangle = \lambda(s) | w_{s} \rangle$ to obtain

$$ \partial_{s} | w_{s} \rangle = \frac{1}{\lambda(s) - F_{\psi}^{K'}(s)} (F_{\psi}^{\perp} - \partial_{s} \lambda(s)) | w_{s} \rangle , $$

(B6)

and then

$$ \| \partial_{s} | w_{s} \rangle \| \leq \max_{0 \leq s \leq 1} 2 \| F_{\psi}^{\perp} \| / \Delta(s) . $$

(B7)

Here, $\Delta(s)$ is the spectral gap between the largest and second largest eigenvalues of $F_{\psi}^{K'}(s)$. In particular, in the perturbative limit where $\| F_{\psi}^{\perp} \| \leq \Delta/4$, $\Delta(s) \geq \Delta/2$ as each eigenvalue of $F_{\psi}^{K'}(s)$ differs from
the eigenvalues of $F^{K'}_\psi$ by, at most, $\Delta/4$. Then, $\Delta(s) = \Omega(\Delta)$. To obtain Eq. (B7), we also used the property $\partial_s \lambda(s) = \langle w_s | F^\perp_\psi | w_s \rangle$. Choosing $\epsilon_D = O(e^{-2\Delta^2/(L\|O\|^2)})$, Eqs. (B3), (B7), and (B5) imply

$$\| |w_1\rangle - |w_0\rangle \| = O(\epsilon) .$$

(B8)

Our choice of $\epsilon_D$ implies $\|F^\perp_\psi\| = O(\epsilon\Delta)$ in Eq. (B3). Note that $\|F^\perp_\psi\| \leq \Delta/4$ for sufficiently small $\epsilon$, justifying the arguments about the perturbative limit.

Equation (B8) implies that, if $V^\dagger$ is the unitary Lie-group transformation that mapped $F_\psi$ to $F^{K'}_\psi$ via the diagonalization procedure, i.e. $F^{K'}_\psi = V^\dagger F_\psi V$, then

$$\| |\psi\rangle - V |w_0\rangle \| = O(\epsilon) .$$

(B9)

This implies that, if the expectation values are known exactly, the diagonalization procedure can be used to obtain a sequence of Lie-group operations that transform a weight state $|w_0\rangle$ to a state that is $O(\epsilon)$-close to the GCS $|\psi\rangle$.

The weight state $|w_0\rangle$ can be transformed to the highest-weight state by a sequence of Lie-group operations referred to as Weyl reflections. To show this, we simply need to show that both, $|w_0\rangle$ and $|hw\rangle$ belong to the orbit of GCSs and thus are connected via a Lie-group transformation. The proof is by contradiction: If $|w_0\rangle$ is not a GCS, then $V |w_0\rangle$ is orthogonal to $|\psi\rangle$ and Eq. (B9) is not satisfied (assuming small $\epsilon$). These Weyl reflections, in addition to the $K'$ unitaries output by the diagonalization procedure, provide a sequence of $K$ simple Lie-group operations to transform $|hw\rangle$ into a state that is $O(\epsilon)$-close to $|\psi\rangle$.

The effects of additional errors from not knowing the expectation values exactly are now analyzed. In the actual case, the starting Hamiltonian is

$$\tilde{F}_\psi = \sum_{m=1}^M O_m (\tilde{O}_m) \psi ,$$

(B10)

where $\langle \tilde{O}_m \rangle \psi$ are estimates of $\langle O_m \rangle \psi$ within precision $\epsilon_M$. (We assume, for simplicity, that all the expectations are known within the same precision.) It follows that

$$\| F_\psi - \tilde{F}_\psi \| = O(M\|O\|\epsilon_M) .$$

(B11)

We will use perturbation theory to make several useful claims about $\tilde{F}_\psi$.

Let $|\tilde{\psi}\rangle$ be the eigenstate of largest eigenvalue of $\tilde{F}_\psi$, which is also a GCS. A similar analysis as the one that resulted in Eq. (B7) for this case implies

$$\| |\psi\rangle - |\tilde{\psi}\rangle \| \leq \frac{2\|F_\psi - \tilde{F}_\psi\|}{\Delta'} ,$$

(B12)

where $\Delta'$ is the minimum spectral gap of the Hamiltonian that continuously interpolates between $F_\psi$ and $\tilde{F}_\psi$. In the perturbative regime where $\|F_\psi - \tilde{F}_\psi\| = O(\epsilon\Delta)$, $\Delta' = \Omega(\Delta)$ and

$$\| |\psi\rangle - |\tilde{\psi}\rangle \| = O(\epsilon) .$$

(B13)

The diagonalization procedure will then be applied to $\tilde{F}_\psi$. To satisfy Eq. (B13), it then suffices to set $\epsilon_M = O(\epsilon\Delta/(M\|O\|))$ in Eq. (B11). The largest and second largest eigenvalues of $\tilde{F}_\psi$ differ from those of $F_\psi$ by an amount of order $\Delta$. Then, the spectral gap of $\tilde{F}_\psi$ is also $\Omega(\Delta)$ and a perturbative analysis also implies that $\epsilon_D = O(e^{-2\Delta^2/(L\|O\|^2)})$ suffices to output a Hamiltonian that is sufficiently close to being diagonal.

Our choice of $\epsilon_D$ determines the number of steps $K'$ for the diagonalization procedure. Let the Hamiltonian at the $K'$-th step be $\tilde{F}^{K'}_\psi = \tilde{F}^{CSA}_\psi + \tilde{F}^\perp$, where $\tilde{F}^{CSA}_\psi \in \mathfrak{h}_D$ and $\tilde{F}^\perp \in \mathfrak{h}^\perp \oplus \mathfrak{h}^-$. We also let $|\tilde{w}_1\rangle$ and $|\tilde{w}_0\rangle$ be the eigenstates of largest eigenvalue of $\tilde{F}^{K'}_\psi$ and $\tilde{F}^{CSA}_\psi$, respectively. Following a similar analysis as the one that led to Eq. (B8), we obtain

$$\| |\tilde{w}_1\rangle - |\tilde{w}_0\rangle \| = O(\epsilon) .$$

(B14)

The desired output of the diagonalization procedure is then $\tilde{F}^{CSA}_\psi$ and the relevant eigenstate is the weight state $|\tilde{w}_0\rangle$. If $\tilde{V}^\dagger$ is the unitary Lie-group transformation that satisfies $\tilde{F}^{K'}_\psi = \tilde{V}^\dagger \tilde{F}_\psi \tilde{V}$, which was obtained via the diagonalization procedure, then

$$\| |\psi\rangle - \tilde{V} |\tilde{w}_0\rangle \| \leq \| |\psi\rangle - |\tilde{\psi}\rangle \| + \| |\tilde{\psi}\rangle - \tilde{V} |\tilde{w}_1\rangle \| + \| \tilde{V} |\tilde{w}_1\rangle - \tilde{V} |\tilde{w}_0\rangle \| .$$

(B15)

Equation (B13), our choice of $\epsilon_D$, and Eq. (B14) imply that each term in the right hand side of Eq. (B15) is $O(\epsilon)$, respectively. In particular,

$$\| |\psi\rangle - \tilde{V} |\tilde{w}_0\rangle \| = O(\epsilon) .$$

(B16)

In summary, when the input to the diagonalization procedure is the Hamiltonian $\tilde{F}_\psi$ obtained from an estimate of the expectation values, the output is a Hamiltonian $\tilde{F}^{CSA}_\psi$ and a Lie-group operation $\tilde{V}$, given as a sequence of exponentials of the form of Eq. (4). The eigenstate of largest eigenvalue of $\tilde{F}^{CSA}_\psi$ is a weight state $|\tilde{w}_0\rangle$, and if acted on by $\tilde{V}$, it outputs a GCS that is $O(\epsilon)$-close to $|\psi\rangle$. A sequence of simple Weyl reflections transforms $|\tilde{w}_0\rangle$ into the highest-weight state. These reflections, together with the unitaries obtained by the diagonalization procedure, provide the unitaries that satisfy Eq. (4).