Variational Quantum Circuits for Multi-Qubit Gate Automata

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Variational quantum algorithms (VQAs) may have the capacity to provide a quantum advantage in the Noisy Intermediate-scale Quantum (NISQ) era. Here, we present a quantum machine learning (QML) framework, inspired by VQAs, to tackle the problem of finding time-independent Hamiltonians that generate desired unitary evolutions, i.e. multi-qubit quantum gates. The Hamiltonians are designed by tuning local fields and two-body interaction terms only. We find that our approach achieves high fidelity quantum gates, such as the Toffoli gate, with a significantly lower computational complexity than is possible classically. This method can also be extended to realize higher-order multi-controlled quantum gates, which could be directly applied to quantum error correction (QEC) schemes.

I. INTRODUCTION

Quantum computing holds the promise of being able to solve some difficult computational problems faster than is possible classically [1, 2]. Recently variational quantum algorithms (VQAs) have emerged as a family of algorithms that could provide a quantum advantage in the Noisy Intermediate-Scale Quantum (NISQ) era [3, 4]. VQAs provide a framework to solve a variety of optimisation [5], linear algebra problems [6], and the prospect of simulating large quantum systems [7–12]. In particular, quantum machine learning has received significant attention as a potentially useful near-term application of VQAs, where the cost function can be efficiently computed by a noisy quantum circuit [13].

Unitary evolution of the form $U(t) = e^{-iHt}$ describes the transformation of a time-independent Hamiltonian Hon a set of qubits. Since scaling the interaction strengths of the Hamiltonian leads to the same dynamics with reciprocally scaled times, we consider these cases equivalent. Therefore, we only consider t=1 for simplicity. The question of whether time-independent Hamiltonians comprising physical (such as two-body) terms can implement useful multi-qubit quantum gates, such as the Fredkin, Toffoli or 3-qubit quantum Fourier transform, and other useful quantum tasks has been an area of recent research interest [14-18], with various classical machine learning and other optimization techniques being deployed. The obvious advantage of the result (the obtained optimized time-independent Hamiltonian) will be in "time-control". The time independent Hamiltonian is simply switched "on" once and then switched "off", and it should accomplish a target unitary gate. We call the collection of qubits evolving according to this Hamiltonian a multi-qubit gate automata. Such automata should be preferable to a sequence of several gates as in a circuit model implementation of the target unitary, as that will naturally involve several on and off processes (one

for each gate).

In most current circuit model approaches for quantum computing, two-qubit gates are implemented using twoqubit interactions at the hardware level and then a multiqubit unitary is synthesized by using a sequence of these and local gates – here we intend to explore beyond this common strategy and seek whether a collection of various two-qubit interactions, kept static and "on" for a certain amount of time, can be directly used to implement a multi-qubit unitary. This problem is not trivial because when one looks at typical useful multi-qubit gates, if they are to be performed naively with a single term time-independent Hamiltonian, then this has to be a multi-qubit interaction, which is not so physical and will be typically difficult to realize on most experimental platforms. A subset, Γ , of interactions should thus be considered, depending on hardware. In most cases, this subset contains only single-term and two-body interactions that could be implemented relatively straightforwardly experimentally. The question of whether a general unitary evolution is possible from such a restricted subset of interactions while avoiding time-dependence (the extreme version of which is a sequence of gates) is highly relevant for quantum simulation of Hamiltonians on quantum computers [19] and large-scale universal quantum computation itself [20, 21], where implementation relies on the capability of performing entangling gates involving multiple qubits with high fidelity. Strategies to directly implement higher-order quantum gates, such as Toffoli gates, have been considered from a quantum control perspective [22–24], and using larger Hilbert spaces with ancillary information carriers [25]. The identification of experimentally-realizable and low-noise alternative strategies for gate synthesis and simulation could be significant for near-term quantum computing architectures because effective multi-qubit gates can implement general quantum circuits more efficiently, i.e. in a lower gate depth [24, 26] (a lower depth is obviously very useful for variational circuits). It is worth highlighting that the framework advanced in this paper differs significantly from techniques such as quantum control for generating multi-qubit gates [24, 27] and quantum gate compi-

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lation [28–30]. Quantum control theory allows for timedependent Hamiltonians, while quantum gate compilation foregoes dealing directly with Hamiltonians, looking instead for sequences of gates whose overall action results in a target operation.

There is, however, a severe bottleneck in the optimization of physical couplings to obtain multi-qubit gate automata that give useful multi-qubit gates. For every choice of variational parameters, the evolution of the multi-qubit system according to a time-independent Hamiltonian has to be computed – a $2^n \times 2^n$ matrix problem for a classical optimizer. Thus techniques used so far [14–18] for designing multi-qubit gate automata cannot be scaled. In this paper, we demonstrate that VQAs can be used to efficiently compute the interaction strengths of the collection of physical (local and twobody) terms constituting the time-independent Hamiltonian for a Toffoli gate, and unitary operations corresponding to higher-order many-body qubit interactions with high fidelity. Not only is there a computational complexity reduction by optimizing the couplings of the automata through a quantum circuit, for the examples we study, we also find that it actually leads to better, more optimal, results than has been found previously though classical optimizations. Trotterization, even to low order, still has sufficiently low errors that it is ideal for implementation in a gate-based VQA circuit. The basic idea is that we optimize the couplings required in the hardware through a gate-based VQA circuit and then use the results to design the hardware automata where quibits are coupled according to the optimal strengths obtained from the VQA.

VARIATIONAL QUANTUM ALGORITHMS

Fault-tolerant quantum computers could still be many years, or even decades, away [3]. In the near-term, a key question for quantum computing is whether there are useful applications for NISQ devices that offer a quantum advantage. Any practical use case must therefore have a limited number of qubits, limited qubit connectivity, and coherent and incoherent errors that limit quantum circuit depth [31]. Here, VQA plays an important role. Problems that can be solved by VQAs with cost functions that can be efficiently implemented as low-depth quantum circuits offer a route for potential quantum advantage for NISQ devices. VQAs consist of two parts, a quantum processor, where the given problem is addressed via state preparation and unitary operations, and a classical computer with a feedback loop which optimizes the cost that the quantum computer provides.

In general, the initial task of any VQA problem is to prepare a quantum state and then measure the output after applying parameterized unitaries within the quantum processing unit (QPU). The measured outcome is processed through a classical optimization procedure where the updated parameters are sent back to the quantum

processor in order to minimize the cost. The optimization process will continue until the termination condition is met. In our case, the VQA is used to efficiently compute the difference between two different dynamical evolutions. The difference is then minimised in order to find the qubit couplings that implement more complex multi-qubit gates with a single time-independent Hamiltonian. The minimization consists of a cost function that is generated by the Hilbert-Schmidt test. The variational unitary in this problem is named the Hamiltoian Variational Ansatz (HVA) and its structure is dependent on the problem Hamiltonian [32, 33]. Fig. 1 shows the VQA structure we have implemented.

The ansatz of a VQA is important, as is must be able to efficiently encode the solution to the problem of interest. Thus, the specific structure of the ansatz generally depends on the task at hand, where the details of the problem itself are used to tailor the ansatz [34]. In general, a variational ansatz can be expressed as the product of L sequentially applied unitary matrices [35],

$$U(\theta) = \prod_{l=1}^{L} U_l(\theta_l), \tag{1}$$

$$U_l(\theta) = \prod_{k=1}^{K} e^{-i\theta_k H_k} W_k, \tag{2}$$

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where the set of H_k with $k \in \{1, ..., K\}$ is the generator of the variational unitary matrices for each layer; the set of θ_k parameters are optimized classically to find the solution; and the set of W_k are unparameterized gates in each laver.

In general, there can be several ways to design a suitable problem-inspired ansatz, for example, quantum approximate optimization algorithm (QAOA) [36], hardware efficient ansatz [37], quantumoptimal-control-inspired ansatz (QOCA) [38], symmetry motivated ansatze [39] and Hamiltonian variational ansatz (HVA) [32, 33]. In this paper, we use an HVAinspired approach.

In our case, the Hamiltonian terms are at most twobody interactions $\sigma_i^{\alpha} \otimes \sigma_j^{\beta}$, which are Pauli operators applied to spins i and j. In general, the Hamiltonian terms are therefore non-commuting. The Hamiltonian His Trotterized with finite Trotter-Suzuki depth m, each Hamiltonian term is then scaled by a vector of tunable parameters θ , while t is set to 1. The unitary evolution of this circuit would thus be

$$U_{\text{HVA}}(\boldsymbol{\theta}) = \prod_{l=1}^{m} \prod_{j=1}^{Q} e^{-i\theta_j H_j} \approx e^{-iHt},$$
 (3)

where Q is the number of terms in the Hamiltonian H.

Here, we use this efficient state preparation to find the approximate evolution of H and compare its evolution with that of the target quantum gate.

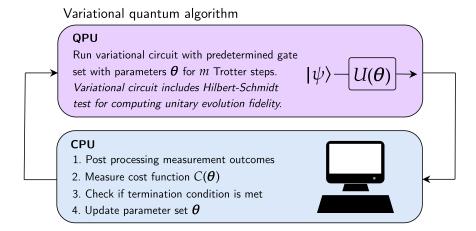


FIG. 1. The VQA structure we have implemented is depicted as a control flow that alternately uses the QPU then CPU until a termination condition is met – the cost $C(\theta)$ is sufficiently small. The Hilbert-Schmidt test circuit used for computing the fidelity is given in Fig. 3.

III. GATE DESIGN PROBLEM

The design of a time-independent Hamiltonian, $H(\theta)$, that generates a target unitary operator, U_{target} , is generally an optimization problem to minimize the distance between $e^{-iH(\theta)}$ and U_{target} . Previously, various numerical methods such as differential evolution and supervised learning have been used [15, 17]. The principal branch of the logarithm for the target unitary gate gives a Hamiltonian that generates the target evolution $H_{\mathrm{principal}} = -iV \log(\Lambda) V^{\dagger}$, with the spectral decomposition $U_{\mathrm{target}} = V \Lambda V^{\dagger}$. Thus, $H_{\mathrm{principal}}$ can be uniquely determined from U_{target} and is denoted as the principal *generator* to distinguish it from other possible generators. In general, it contains physical interactions that can be easily realized in given experimental setups, as well as unphysical interactions that are hard to implement, such as non-local three- or four-qubit interactions. The main goal of the approach proposed in Ref. [17] is to construct a new Hamiltonian with only physical interactions such that $e^{-iH(\theta)t} \approx U_{\text{target}}$. In particular, we consider only local and two-qubit coupling terms. Here, we do not consider ancillary qubits. Thus three conditions are imposed on parameter Hamiltonians:

- 1. $H(\theta)$ contains only physical interactions;
- 2. the Hamiltonian commutator is vanishing, $[H(\boldsymbol{\theta}), H_{\text{principal}}] = 0;$
- 3. the Hamiltonian difference gives terms that do not contribute to the unitary evolution, $\operatorname{Eig}(H(\boldsymbol{\theta}) H_{\operatorname{principal}}) = \{2\pi n_i\}$ for $(n_i \in \mathbb{Z})$.

The above three conditions simplify the problem of gate synthesis. Physical parameter sets for the Fredkin gate and Toffoli gate have been found [17]. Although optimal parameters for a fidelity greater than 0.99 was achieved for the Fredkin gate, for the Toffoli gate the

greatest fidelity was only about 0.98 – potentially due to the computational complexity of the full supervised learning approach.

Here, we propose a simple variational circuit approach to reduce the computational complexity, even for classical simulation, and find a fidelity greater than 0.99 for the Toffoli gate. This approach allows quantum gates with higher numbers of qubits to be realised, and we show results for a 4-qubit parity check.

IV. TIME-INDEPENDENT HAMILTONIANS FOR MULTI-QUBIT GATES

The most general Hamiltonian, $H(\boldsymbol{\theta}) = \sum_{j=1} H_j(\theta_j)$, with at most two-qubit interaction terms can be written

$$H(\boldsymbol{h}, \boldsymbol{J}) = \sum_{i} h_{i}^{\alpha} \sigma_{i}^{\alpha} + \sum_{i,j} J_{i,j}^{\alpha,\beta} \sigma_{i}^{\alpha} \sigma_{j}^{\beta}, \tag{4}$$

where $(h, J) = \theta$ becomes the parameter set for the variational quantum circuit. For our imposition of a *physical* gate set, we require $\alpha = \beta$, such that the interactions between spins at their most complex are XYZ Heisenberg interactions.

The parameter set $\boldsymbol{\theta}$ is found using the HVA-inspired variational hybrid approach. The Trotter-Suzuki method is used to build the quantum circuit from the individual Hamiltonian terms. With m Trotter steps, Q terms in the Hamiltonian, and t=1, the evolution becomes

$$U(\boldsymbol{\theta}) = e^{-iH(\boldsymbol{\theta})} = \left(\prod_{j=1}^{Q} e^{-iH_j(\theta_j)/m}\right)^m + O(\frac{Q^2}{m^2}). \quad (5)$$

The quantum circuit is therefore equal to the consecutive implementation of all individual two-qubit Hamiltonian terms rescaled by a prefactor 1/m. An Ising

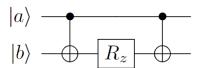


FIG. 2. Circuit to implement the evolution of the Ising ZZ interaction, $\sigma_i^z \sigma_j^z$, between qubits i and j. The XX and YY interactions can be similarly implemented with a simple basis transformation at the beginning and end of the circuit.

interaction term between qubits i and j, $\sigma_z^z \sigma_j^z$, is implemented straightforwardly with the circuit shown in Fig. 2. The quantum circuit corresponds to the evolution $U_{\rm QC}(\boldsymbol{\theta}) = \prod_{j=1}^Q e^{-iH_j(\theta_j)}$. For large enough m, the error term of the evolution in Eq. (5) is small and we have $U(\boldsymbol{\theta}) \approx U_{\rm QC}(\boldsymbol{\theta})$.

In the supervised machine learning approach to this problem [17], the figure of merit that determines the cost function involves the fidelity of the parameterized state evolution, $e^{-iH(\theta)}|\psi\rangle$, with the target evolution of the quantum state, $F(\psi) = \langle \psi | U_{\rm target}^{\dagger} e^{-iH(\theta)} | \psi \rangle$. The cost function is the average fidelity, F, for all possible states $|\psi\rangle$ – of course, in practice, only a large sample of random states is chosen. The fidelity is maximised during the supervised machine learning procedure.

In the variational approach, we use an operator fidelity measure, $F(\boldsymbol{\theta}) = \text{Tr}\left[U_{\text{target}}^{\dagger}U_{QC}(\boldsymbol{\theta})\right]/2^n$, for n qubits. The quantum circuit therefore only finds an approximate fidelity $\tilde{F}(\boldsymbol{\theta})$. The cost function uses this fidelity

$$C(\boldsymbol{\theta}) = 1 - \frac{1}{2^{2n}} \left| \text{Tr} \left[U_{\text{target}}^{\dagger} U_{\text{QC}}(\boldsymbol{\theta}) \right] \right|^2.$$
 (6)

The cost in Eq. (6) can be efficiently obtained directly using the Hilbert-Schmidt (HS) test [28], see Fig. 3. It requires 2n qubits, where on the first n qubits the evolution $U_{QC}(\boldsymbol{\theta})$ is applied, while on the next n qubits, the target unitary gate, U_{target} , using one of its known implementations using an array of quantum gates (for example, for the Toffoli gate, 5 two qubit gates can be used along with local gates [40]; for other multi-qubit unitaries, an implementation in terms of a series of quantum gates can itself be generated, for example, by variational circuit optimization [28–30] – we will target unitary operations that have an efficient, i.e., polynomial, circuit implementation). The two subsystems on which both unitaries act are first maximally entangled (2n gates). After both sets of gates are applied to each subsystem separately, a global Bell state measurement (another 2ngates) is performed to obtain the overall average fidelity $\left| \operatorname{Tr} \left[U_{\operatorname{target}}^{\dagger} U_{\operatorname{QC}}(\boldsymbol{\theta}) \right] \right|^2 / d^2$. After the calculation of the $\cos t$, a new θ is trialled. For this, the gradient must be computed, which can be performed efficiently on a classical computer using the parameter-shift method [41]. For larger n we will use the local Hilbert-Schmidt norm as described in Ref.[28].

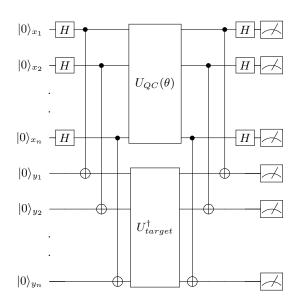


FIG. 3. The Hilbert-Schmidt (HS) test. Two unitaries $U_{QC}(\theta)$ and U_{target}^{\dagger} are acting on n qubit basis states. Measuring all the 2n qubits in $|0\rangle$ state will give the output $|\text{Tr}\left[U_{\text{target}}^{\dagger}U_{\text{QC}}(\boldsymbol{\theta})\right]|^2/2^{2n}$ and thus we can efficiently compute the cost in Eq. (6).

A. Quantum Toffoli gate

We first demonstrate the ability to find an optimal time-independent Hamiltonian with single and two qubit terms that implements the Toffoli gate. For just m=6 Trotter steps, the unitary evolution quickly finds a minimum parameter set θ_{\min} , such that $C(\boldsymbol{\theta})$ is close to 0, see Fig. 4. Remarkably, even for a low m Trotter steps, the operator fidelity gives $F(\boldsymbol{\theta}_{\min}) > 0.99$, see Fig. 4. The interactions found for the Toffoli gate are presented in Fig. 5(a).

Apart from 3-qubit gate like Toffoli, our approach can also be applied to realize the evolution of more complicated interactions, such as the parity of multi-qubit systems.

B. Parity gate

An extension of the variational quantum optimization algorithm is to see whether a parity check procedure, to detect possible errors in the surface code, can be implemented directly by a time-independent Hamiltonian. Assuming three qubits with computational-basis states $z_i \in \{0,1\}$ with i=1,2,3, the evolution at $t=\pi/4$ of the interaction $P=\sigma_1^z\otimes\sigma_2^z\otimes\sigma_3^z\otimes\sigma_4^y$ can be used to

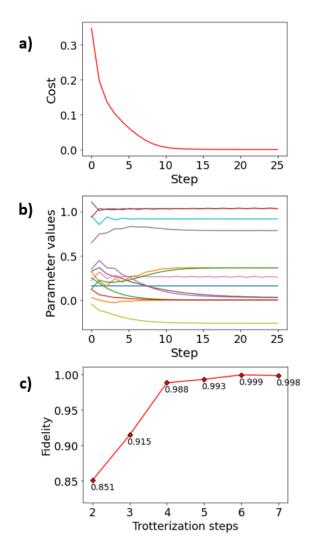
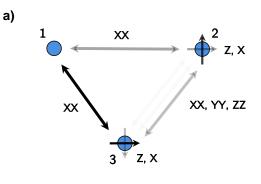


FIG. 4. (a) shows training data of the cost optimization for a total Trotter steps m=6, with gradient descent optimizer, where the optimizer reaches the minimum after the first few steps. (b) plots the evolution of the parameters with the optimization steps. All of the parameters saturate after a few steps. (c) shows the improvement of fidelity between U_{Toff} and $e^{-iH(\theta_{\text{opt}})}$, for t=1, as a function of the number of Trotter steps where θ_{opt} is the set of optimal parameters in the parameterized Hamiltonian of Eq. (4) for each number of Trotterization steps.

measure the parity $p = z_1 \oplus z_2 \oplus z_3$,

$$U(\frac{\pi}{4})|z_1 z_2 z_3\rangle|0\rangle = \frac{1}{\sqrt{2}} (|z_1 z_2 z_3\rangle|0\rangle + iP|z_1 z_2 z_3\rangle|0\rangle)$$
(7)
= $\frac{1}{\sqrt{2}}|z_1 z_2 z_3\rangle (|0\rangle - (-1)^p|1\rangle),$ (8)

where $U(\frac{\pi}{4}) = e^{-iP\frac{\pi}{4}}$. The state of the last qubit is either $|+\rangle$ or $|-\rangle$ depending if the parity p is even or odd respectively. We can then perform an x-basis measurement by applying a Hadamard to the last qubit followed by a computational basis measurement. The measurement outcome of the final qubit thus corresponds to the



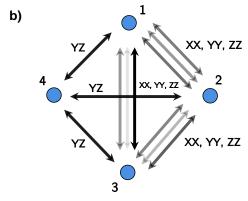


FIG. 5. Interaction diagrams with single and two-qubit interactions for (a) Toffoli gate and (b) Parity gate. All the parameters are found from variational circuit optimization and give fidelities of F>0.99. The Trotter steps used are m=6 for (a) and m=5 for (b). The interaction strengths for (a): $J_1^x=1.09,\ J_1^z=2.35,\ J_2^x=3.11,\ J_2^z=-0.78,\ J_{12}^{xz}=0.07,\ J_{12}^{yy}=0.07,\ J_{12}^{zz}=0.78,\ J_{13}^{xx}=1.089,\ J_{23}^{zz}=3.11.$ Interaction strengths for (b): $J_{12}^{xx}=1.42,\ J_{12}^{yy}=1.04,\ J_{12}^{zz}=1.30,\ J_{23}^{xx}=1.23,\ J_{23}^{yy}=0.73,\ J_{23}^{zz}=1.60,\ J_{13}^{xx}=1.03,\ J_{13}^{yy}=0.29,\ J_{13}^{zz}=2.57,\ J_{24}^{zy}=2.37,\ J_{14}^{zy}=2.29,\ J_{34}^{zy}=2.30.$

parity of the first three qubits. Fig. 5(b) shows the singlequbit and two-qubit interactions required to perform the three-qubit parity check evolution with a fidelity of more than 0.99.

V. COMPLEXITY OF THE ALGORITHM

The problem-inspired Ansatz is dependent on the target unitary evolution. However, we can bound the scaling of the computational complexity by the worst case for the number of physical interactions. First we consider the $U_{\rm QC}(\theta)$ part of the algorithm. For quantum complexity, we consider the number of two-qubit interaction terms, two-qubit gates, and ignore the number of local gates as they can implemented arbitrarily fast. The general parameterized Hamiltonian of Eq. (4) can be represented by nine graphs, one for each of the possible $\sigma_i^{\alpha} \otimes \sigma_j^{\beta}$ between qubits i and j. The worst case is thus a complete interaction graph for each. The number of edges in the complete graph scales as n(n-1)/2.

Hence, for the complete set of two-qubit gates, we find 9n(n-1)/2. However, this is only the complexity of a single Trotter step. The complexity is $O(mn^2)$ for m Trotter steps. Assuming m is constant as n increases, and it does not decrease the fidelity significantly, the complexity is $G(n) = O(n^2)$. However, m can scale as poly(n) with the number of qubits [42]. Similarly the implementation of $U_{\rm target}^{\dagger}$ is efficient (we can only seek to find our automata couplings through our VQA method for such types of unitaries).

The overall complexity of the parameterized quantum circuit must include the complexity of the cost function. The cost function of Eq. (6) is computed using the Hilbert-Schmidt test of Fig. 3, which has a gate complexity that scales as $O(n^2)$ for n qubits. Thus, the overall quantum circuit for our variational quantum circuit also scales as $O(n^2)$. Classically, the complexity of computing the natural dynamical evolution from an engineered Hamiltonian is due to the complexity of exponentiation of a matrix, which scales as $O(N^3) = O(2^{3n})$ [43]. Therefore, even if m scales as $\operatorname{poly}(n)$, we still find a significant (exponential) complexity advantage in using the variational quantum approach for realizing multi-qubit quantum gates.

VI. DISCUSSION

We have shown that variational quantum optimization can find the coupling parameters for multi-qubit quantum gates more efficiently than a classical supervised learning approach. Besides the Toffoli gate, using variational quantum optimization, we have shown that we can realize a unitary that results from a multi-qubit interaction solely using two-body time-independent Hamiltonian terms, namely the parity gate in Section. IV B, which could find use in quantum error correction [44, 45].

While our demonstrations have only been in terms of designing Hamiltonians in 3 and 4 qubit systems, the problem should scale well for designing automata for multiqubit gates involving a larger number of qubits. As it is a variational quantum circuit based method, it is possible that barren plateaus [46, 47] and local minima may appear for larger numbers of qubits, but in our specific examples they did not. For the Hilbert-Schmidt norm cost function, for a larger number of qubits one can use the local Hilbert-Schmidt test to avoid plateaus therein [28]. Additionally, our ansatz is problem inspired, and we impose certain conditions to our Hamiltonian so that we are able to reduce the variational parameters we start with. One could perhaps use inductive techniques – optimal values of couplings derived for gates for smaller numbers of qubits could be used to formulate the initial ansatz for a larger number of qubits. Our protocol is an example of an application of VQAs for an useful task within the field of quantum computation itself. The results will be useful in creating hardware of permanently interacting qubits which will enact multi-qubit quantum gates with time independent Hamiltonians, thereby alleviating the complexity of time control. On the other hand, the results themselves (the multi-qubit gates performed as an automata in the above sense), can be part of new ansatze for variational circuits (as these new gates become hardware feasible), which increases their scope in parameter space and may well alleviate some their problems and quantum computation in general by reducing depth.

VII. ACKNOWLEDGEMENTS

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