Variational learning of Grover's quantum search algorithm

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Given a parametrized quantum circuit such that a certain setting of these real-valued parameters corresponds to Grover's celebrated search algorithm, can a variational algorithm recover these settings and hence learn Grover's algorithm? We studied several constrained variations of this problem and answered this question in the affirmative, with some caveats. Grover's quantum search algorithm is optimal up to a constant. The success probability of Grover's algorithm goes from unity for two qubits, decreases for three and four qubits, and returns near unity for five qubits, then oscillates ever so close to unity, reaching unity in the infinite qubit limit. The variationally approach employed here found an experimentally discernible improvement of 5.77% and 3.95% for three and four qubits, respectively. Our findings are interesting as an extreme example of variational search, and they illustrate the promise of using hybrid quantum classical approaches to improve quantum algorithms. This paper further demonstrates that to find optimal parameters, one does not need to vary over a family of quantum circuits to find an optimal solution. This result looks promising and points out that there is a set of variational quantum problems with parameters that can be efficiently found on a classical computer for an arbitrary number of qubits.

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Grover's algorithm [1] is one of the most celebrated quantum algorithms, enabling quantum computers to quadratically outperform classical computers in a database search, provided database access is restricted to a "black box"—called the oracle model. In addition to the wide application scope of a database search, Grover's algorithm has further applications as a subroutine used in a variety of other quantum algorithms.

Variational hybrid quantum-classical algorithms have recently become an area of significant interest [2–9]. These algorithms have shown several advantages, such as robustness to quantum errors and low coherence time requirements [10], which make them ideal for implementations in current quantum computer architectures. Here we take inspiration from algorithms such as the variational quantum eigensolver (VQE) [2] and the quantum approximate optimization algorithm (QAOA) [3]. The general procedure of these variational hybrid quantum and/or classical algorithms is the following:

(i) Prepare state $|\psi(\theta)\rangle$ using a quantum computer, where $\theta = (\theta_1, \theta_2, \ldots, \theta_k)$ are tunable parameter(s). The state is prepared by specifying a sequence of k gates $\mathcal{U}^{(1)}(\theta_1)\mathcal{U}^{(2)}(\theta_2)\cdots\mathcal{U}^{(k)}(\theta_k)$ applied to a starting reference state $|r\rangle$. Thus, the prepared state is $|\psi(\theta)\rangle = \mathcal{U}^{(1)}(\theta_1)\mathcal{U}^{(2)}(\theta_2)\cdots\mathcal{U}^{(k)}(\theta_k)|r\rangle$.

(ii) Measure the expectation value of an objective function $\langle A(\theta)\rangle$. The objective function will depend on the problem to be solved. In the case of VQE, the interest is in finding the eigenvalues of a given Hamiltonian. Moreover, the quantum computer is used to calculate the expectation values of the separate terms in the Hamiltonian. For QAOA, the objective function approximates the solution of an optimization problem (for details, see [3]). The expectation value of this objective function can be calculated using a quantum computer, but it can also be efficiently evaluated classically.

(iii) Using a classical computer and an optimization algorithm, find new parameters θ' that minimize $\langle A(\theta)\rangle$. Having found the new parameters, iterate.

Here we consider a variational approach to the established problem of Grover's search [1]. Note that Grover's search was generalized to the setting of adiabatic quantum computing in [11,12]. Grover's quantum search algorithm has been shown to be asymptotically optimal [13–15] and hence provides a limiting test case in which to apply contemporary variational hybrid quantum and/or classical algorithms.

We apply a variational algorithm to see if we can recover Grover's algorithm under several constraining scenarios. We motivate our study by recalling that sequencing two Hermitian projectors (Hamiltonians) can be used to recover Grover's search algorithm exactly. We then constrain the search space. For example, in one scenario we fix the oracle—as is standard—to apply a phase factor of -1 to the marked item when varying the time the diffusion generator is applied. In another scenario, we allow the oracle and the diffusion to take the same angle in all iterations. The main objective is to see if a variational algorithm is capable of recovering Grover's algorithm given different restrictions. A peculiar finding is an experimentally discernible improvement of 5.77% and 3.95% for three and four qubits, respectively (compared to Grover's search algorithm).

I. PROBLEM STATEMENT

Let n be the number of qubits and let $N = 2^n$ be the size of the search space. We are searching for a particular

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bitstring $\boldsymbol{\omega} = \omega_1, \omega_2, \omega_3, \ldots, \omega_n$. We define a pair of rank-1 projectors,

$$P_{\boldsymbol{\omega}} = |\boldsymbol{\omega}\rangle\langle\boldsymbol{\omega}|, \tag{1}$$

$$P_{+} = |+\rangle\langle+|^{\otimes n} = |\boldsymbol{s}\rangle\langle\boldsymbol{s}|, \tag{2}$$

where $|\boldsymbol{s}\rangle = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{x}\in\{0,1\}^n}|\boldsymbol{x}\rangle$. To find $|\boldsymbol{\omega}\rangle$, we consider first an ansatz formed by sequencing operators defined in (6) and (7). These operators prepare a state $|\varphi(\boldsymbol{\alpha},\boldsymbol{\beta})\rangle$, defined in (5), with vectors $\boldsymbol{\alpha} = \alpha_1, \alpha_2, \ldots, \alpha_p$ and $\boldsymbol{\beta} = \beta_1, \beta_2, \ldots, \beta_p$. We seek to minimize the orthogonal complement of the subspace for the searched string (3),

$$P_{\boldsymbol{\omega}^\perp} = \mathbb{1} - P_{\boldsymbol{\omega}}. \tag{3}$$

We sometimes call (2) the driver Hamiltonian or diffusion operator [5]. The state is varied to minimize this orthogonal component (4),

$$\min_{\boldsymbol{\alpha},\boldsymbol{\beta}} \langle\varphi(\boldsymbol{\alpha},\boldsymbol{\beta})|P_{\boldsymbol{\omega}^\perp}|\varphi(\boldsymbol{\alpha},\boldsymbol{\beta})\rangle \geqslant \min_{|\phi\rangle}\langle\phi|P_{\boldsymbol{\omega}^\perp}|\phi\rangle. \tag{4}$$

To prepare the state, we develop the sequence (5),

$$|\varphi(\boldsymbol{\alpha},\boldsymbol{\beta})\rangle = \mathcal{K}(\beta_p)\mathcal{V}(\alpha_p)\cdots\mathcal{K}(\beta_1)\mathcal{V}(\alpha_1)|\boldsymbol{s}\rangle, \tag{5}$$

where the operators are defined as (6) and (7),

$$\mathcal{V}(\alpha) := e^{\imath\alpha P_{\boldsymbol{\omega}}}, \tag{6}$$

$$\mathcal{K}(\beta) := e^{\imath\beta P_{+}}. \tag{7}$$

The length of the sequence is $2p$ for integer p. We consider the following problems that the variational algorithm will face.

Problem I.1: Standard oracle, variational diffusion. Find p angles $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)$ and fix $\boldsymbol{\alpha} = (\alpha_1 = \pi, \ldots, \alpha_p = \pi)$ to minimize (4) via the sequence (5), given the operators (6) and (7).

In this problem, we have fixed the standard black-box oracle of Grover's algorithm, and the algorithm optimizes for the angles in the diffusion operator. We also consider a restricted variational problem where all the diffusion operators must apply the same variational angle.

Problem I.2: Standard oracle, restricted variational diffusion. As in problem I.1, except find p angles $\boldsymbol{\beta} = (\beta, \ldots, \beta)$ and choose $\boldsymbol{\alpha} = (\alpha_1 = \pi, \ldots, \alpha_p = \pi)$.

A third problem to which we will apply the variational algorithm is considering both the oracle and the diffusion angles as variational parameters. We consider in this case a phase-matching condition, meaning that angles are restricted so they are equal.

Problem I.3: Restricted variational oracle and diffusion. As in I.1, except find $2p$ angles $(\boldsymbol{\alpha},\boldsymbol{\beta}) = (\alpha_1, \ldots, \alpha_p, \beta_1, \ldots, \beta_p)$ with the restriction $\boldsymbol{\beta} = \boldsymbol{\alpha} = \alpha_1, \alpha_2, \ldots, \alpha_p$ and $\alpha_1 = \alpha_2 = \cdots = \alpha_p$.

Finally, we consider variations of the oracle angles and the diffusion operator separately.

Problem I.4: Variational oracle and diffusion. As in problem I.1, except find $2p$ angles $(\boldsymbol{\alpha},\boldsymbol{\beta}) = (\alpha_1, \ldots, \alpha_p, \beta_1, \ldots, \beta_p)$.

Note that the angles obtained in (4) only minimize the selected cost function for a particular number of qubits. Once the number of qubits changes, the angles obtained in the minimization do not necessarily give the highest probability to find the searched item. Also, it is important to note that these angles are independent of $\boldsymbol{\omega}$. If we fix the number of qubits in the problem and run the algorithm with a particular set of angles, then these angles give the same probability regardless of the $\boldsymbol{\omega}$ we are seeking. As stated earlier, our objective in this work is to see if variational algorithms are able to recover Grover's algorithm. For this purpose, we need a way of comparing both algorithms.

To compare these variational algorithms with Grover's algorithm, consider the variational ansatz case for $p = 1$. Here we recover Grover's operators as the optimal solution for finding a particular string. To prove this, first note that there is only one pair of angles (α, β), so we consider (6) and (7) directly. Since $|\boldsymbol{\omega}\rangle\langle\boldsymbol{\omega}|$ is a projector, we can expand (6),

$$\begin{aligned}\mathcal{V}(\alpha) = e^{\imath\alpha|\boldsymbol{\omega}\rangle\langle\boldsymbol{\omega}|} &= \mathbb{1} + (e^{\imath\alpha} - 1)|\boldsymbol{\omega}\rangle\langle\boldsymbol{\omega}| \\ &= \mathbb{1} - (e^{\imath\widetilde{\alpha}} + 1)|\boldsymbol{\omega}\rangle\langle\boldsymbol{\omega}|,\end{aligned} \tag{8}$$

where in the last step we have defined $\widetilde{\alpha} = \alpha - \pi$. Now we expand the unitary for the driver Hamiltonian (9),

$$\begin{aligned}\mathcal{K}(\beta) &= e^{\imath\beta|\boldsymbol{s}\rangle\langle\boldsymbol{s}|} \\ &= H^{\otimes n}[\mathbb{1} + (e^{\imath\beta} - 1)|\boldsymbol{0}\rangle\langle\boldsymbol{0}|]H^{\otimes n} \\ &\sim H^{\otimes n}[-\mathbb{1} + (e^{\imath\widetilde{\beta}} + 1)|\boldsymbol{0}\rangle\langle\boldsymbol{0}|]H^{\otimes n} \\ &= (e^{\imath\widetilde{\beta}} + 1)|\boldsymbol{s}\rangle\langle\boldsymbol{s}| - \mathbb{1},\end{aligned} \tag{9}$$

where $\sim$ relates the equivalence class of operators indiscernible by a global phase, H is the Hadamard gate, and $\widetilde{\beta} = \beta - \pi$. Notice that for $\widetilde{\alpha} = \widetilde{\beta} = 0$, Grover's oracle and diffusion operators are recovered.

To see that the variational search includes Grover's operators for the case $p > 1$, let us impose $\alpha_1 = \alpha_2 = \cdots = \alpha_p$ and $\beta_1 = \beta_2 = \cdots = \beta_p$. In Figs. 4(a) and 4(b), the circuits for the oracle and the diffusion operator, respectively, are shown. If i pairs of operators (6) and (7) are applied to the initial state $|\boldsymbol{s}\rangle$ as in (5), then we write the prepared state as (10),

$$|\varphi_i\rangle = A_i\frac{1}{\sqrt{N-1}}\sum_{x\neq\boldsymbol{\omega}}|x\rangle + B_i|\boldsymbol{\omega}\rangle. \tag{10}$$

We can relate the amplitudes of one step with the amplitudes of the next step with a recursion such as those that appear in (13) and (14); we express the effect of the operators for the variational search over the state as a matrix (11),

$$\begin{pmatrix} 1 + \frac{a(N-1)}{N} & -a(b+1)\frac{\sqrt{N-1}}{N} \\ -a\frac{\sqrt{N-1}}{N} & (b+1)(1+\frac{a}{N}) \end{pmatrix}. \tag{11}$$

Here $a = e^{\imath\alpha} - 1$ and $b = e^{\imath\beta} - 1$. Notice that for $a = b = -2$ the same relation between amplitudes at different steps in (13) and (14) up to a global phase in the definition of the Grover operators is obtained. Thus, the variational search space includes Grover's original algorithm. From this matrix,

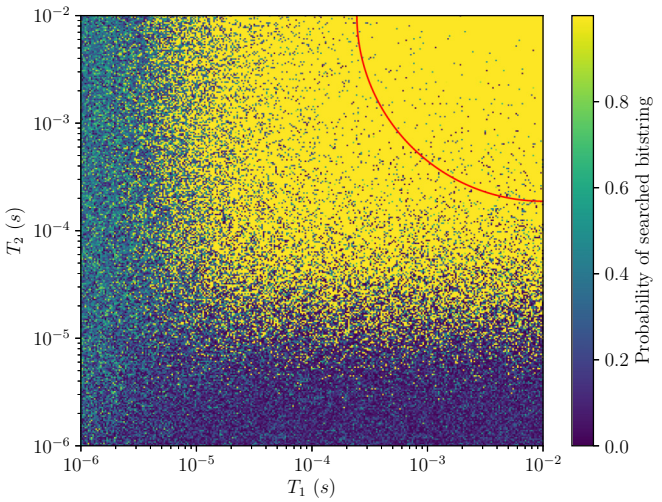


FIG. 1. Probability for finding the solution to the search problem in the case of three-qubit search under T_1 and T_2 noise using variational search. The red circumference in the plot corresponds to a fit circle defined such that the probabilities inside the circle are, on average, larger than 5% of the optimal probability obtained with Grover's algorithm.

it is also possible to see that if the target state is changed, then the angles found through the variational algorithm will give the same probabilities.

An arbitrary phase applied by the oracle was first proposed in [16], although only remarks regarding the use of an arbitrary phase to get higher probabilities for the searched item were made. Afterward, several studies regarding the validity of replacing Grover's oracle and diffusion operator with an arbitrary phase version were performed [17–20]. The main conclusion is that a phase-matching condition is required. This condition, roughly stated, requires the arbitrary angles in the oracle and the diffusion operator to be approximately equal. To address this, we consider also in this work the problem shown in definition I.3, requiring that the variational angles be equal.

II. RESULTS

We have compared the performance of the variational search algorithm to Grover for different numbers of qubits and for the problems I.1, I.2, I.3, and I.4. Surprisingly, in problems I.1, I.3, and I.4 it was found that for a small number of qubits and for the same number of operator applications (or oracle calls) p on which Grover obtains the greatest probability, the variational algorithm achieves greater probabilities for finding the searched string (see Fig. 1). This advantage for a low number of qubits can be seen in Fig. 2. The same plot is obtained for the variational algorithm defined for problems I.1, I.3, and I.4. In Fig. 3 we show the difference between the maximum probabilities of successfully finding the string between Grover's algorithm and the variational approach up to 11 qubits. As the number of qubits grows, there are diminishing oscillations in this difference, in agreement with the fact that Grover is asymptotically optimal. These diminishing oscillations go to zero very quickly after 10 qubits.

In the case of problem I.2, we find through numerics that the advantage over Grover's algorithm is lost. We also show in Table I, for the variational problem I.3, the percentage increase between the variational algorithm and Grover's for the probabilities at the number of oracle calls on which this probability is maximal from two to six qubits. For higher numbers of qubits this difference becomes negligible, although there are small oscillations. The same numbers are obtained (except the angle) for the algorithms in problems I.1 and I.4. We show in Fig. 2 the probability for finding the solution as a function of the only angle and number of qubits when considering the algorithm of problem I.3. In the case of problem I.1, we recover the same probabilities for the marked state as in Grover's algorithm, without the small improvement. From the matrix in (11) and imposing $a = b$ it is possible to plot the probability as a function of the variational angle α and the number of qubits for the algorithm in problem I.3. We show this plot for three to six qubits in Fig. 2.

The local maximum at π is clearly seen at $n = 3$ qubits, but also at this or more qubits this angle is not the global maximum. The variational search manages to find these global maxima by using the basin hopping method [21] for

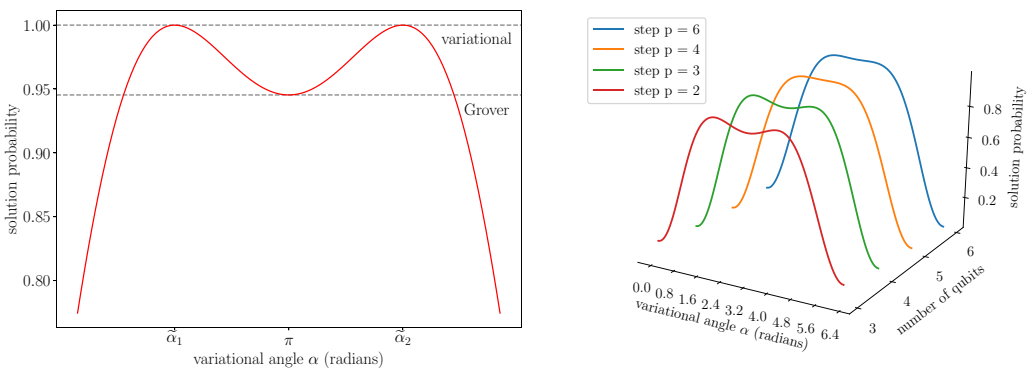


FIG. 2. Left: Grover's algorithm takes a saddle point between two hills. Variational search recovers the hill peaks. Note that the valley becomes increasingly less pronounced past four qubits, providing a negligible range for improvement. Right: probability as a function of the variational angle for the three-qubit case. Grover's algorithm is recovered in the case $\alpha = \pi$; the variational algorithm obtains angles $\widetilde{\alpha}_1 = 2.12^{\text{rad}}$ and $\widetilde{\alpha}_2 = 2\pi - \widetilde{\alpha}_1$.

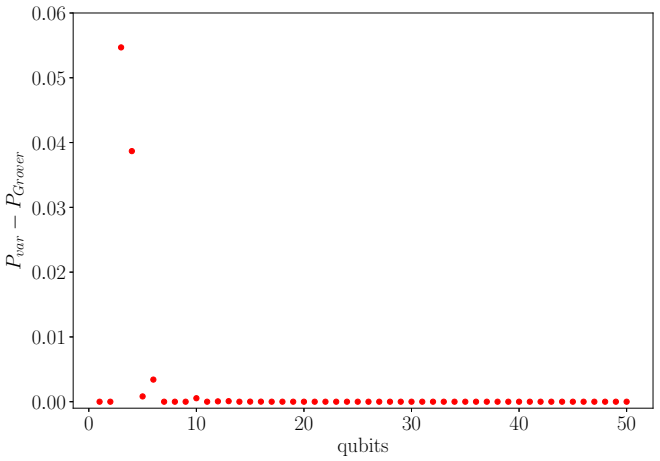


FIG. 3. Difference between variational and Grover. As the number of qubits grows, there are exponentially diminishing oscillations in this difference. Each probability is defined for the optimal step in Grover's algorithm for the number of qubits.

optimization (the search space of the angle is bounded since we restrict to $\alpha \in [0, \pi]$). The difference of the probabilities to find the solution between the original Grover's algorithm and the variational search does not diminish monotonically with the number of qubits. The same results are obtained for problems I.1, I.3, and I.4. In the case of problem I.2, the difference is negligible.

For low $N = 2^n$, where n is the number of qubits in the search, the variational search provides sequences that are more likely to succeed in finding the solution than Grover's algorithm. Grover's algorithm has been proven to be optimal. This slight advantage of the variational algorithm over Grover's is possible since the proofs have considered a large number of qubits [13–15]. We show in the following that this advantage disappears for large N.

To prove this, we first consider the following theorem:

Theorem II.1. The maximum probability achievable for the target state in Grover $\to 1$ as $N \to \infty$.

Before proving this, we present proof of a proposition from Zalka [15].

Proposition II.2. For $N \gg 1$, the probability of measuring the target state $|\boldsymbol{\omega}\rangle$ after making p oracle calls in Grover's algorithm is $P_p = \sin^2(p\phi + \phi/2)$.

TABLE I. Percentage increase between the highest probability for finding the solution after measurement obtained in Grover and the two-level variational ansatz. Percent given as a function of $N = 2^n$, where n is the number of qubits, and at step $p_{\max}$, on which the probability of finding the solution string is maximum. The same table is obtained for the variational ansatz with one angle or with $2p$ angles. Both the diffusion and the oracle use the same angle.

N	$100 \times (P_{\text{variational}} - P_{\text{Grover}})/P_{\text{Grover}}$	Step $p_{\max}$	Angle
2^3	5.77%	2	2.12^{rad}
2^4	3.95%	3	2.19^{rad}
2^5	0.08%	4	2.76^{rad}
2^6	0.34%	6	2.60^{rad}

Proof of proposition II.2. We denote the state of the system for step i of Grover's algorithm as $|\psi_i\rangle$, and the target state is denoted $|\boldsymbol{\omega}\rangle$. As an initial state for the algorithm, we have $|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle$. Following [15], we write the state of the system in the ith state (12) with (13) and (14),

$$|\psi_i\rangle = A_i \frac{1}{\sqrt{N-1}} \sum_{x \neq \boldsymbol{\omega}} |x\rangle + B_i |\boldsymbol{\omega}\rangle, \tag{12}$$

$$A_{i+1} = \left(1 - \frac{2}{N}\right) A_i - 2\frac{\sqrt{N-1}}{N} B_i, \tag{13}$$

$$B_{i+1} = 2\frac{\sqrt{N-1}}{N} A_i - \left(1 - \frac{2}{N}\right) B_i. \tag{14}$$

This can be written as the result of applying a rotation [15] with $\cos(\phi) = 1 - \frac{2}{N}$ and $\sin(\phi) = 2\frac{\sqrt{N-1}}{N}$. For the proof of the theorem, we are interested in the large-N limit. Let us consider then $N \gg 1$, thus $\phi \approx \sin\phi \approx \frac{2}{\sqrt{N}}$. The initial state can be written in terms of this angle,

$$|\psi_0\rangle = \cos(\phi/2) \frac{1}{\sqrt{N-1}} \sum_{x \neq \boldsymbol{\omega}} |x\rangle + \sin(\phi/2) |\boldsymbol{\omega}\rangle.$$

After applying a rotation with angle ϕ, p times (equivalent to applying both operators p times) if $N \gg 1$, then

$$|\psi_i\rangle = \cos(\phi/2 + p\phi) \frac{1}{\sqrt{N-1}} \sum_{x \neq \boldsymbol{\omega}} |x\rangle + \sin(\phi/2 + p\phi) |\boldsymbol{\omega}\rangle.$$

Hence, the probability of measuring $|\boldsymbol{\omega}\rangle$ after p steps is (15),

$$P_p = \sin^2(p\phi + \phi/2). \tag{15}$$

With this, now we prove theorem II.1.

Proof of theorem II.1. From (15) we can calculate the maximum for the probability in the segment $[0, \pi)$. What we actually need is to calculate $p_{\max}$ for which the probability is maximum in said segment. We know there is a maximum at $\pi/2$, thus

$$p_{\max}\phi + \phi/2 = \frac{\pi}{2} \Rightarrow p_{\max} = \frac{\pi}{2\phi} - \frac{1}{2}.$$

Then, for $N \gg 1$ we have

$$p_{\max} = \frac{\pi\sqrt{N}}{4} - \frac{1}{2}. \tag{16}$$

Recall that p represents the oracle calls, thus it must be an integer. Then the maximum must be either (17) or (18),

$$p_{\max} = \left\lfloor \frac{\pi\sqrt{N}}{4} - \frac{1}{2} \right\rfloor, \tag{17}$$

$$p_{\max} = \left\lfloor \frac{\pi\sqrt{N}}{4} - \frac{1}{2} \right\rfloor + 1. \tag{18}$$

We want to prove that as $N \to \infty$, the maximum probability goes to 1. That is, we want to prove $\lim_{N\to\infty}(p\phi + \phi/2) = \pi/2$. We prove this with the following limit (19)—we can

replace (17) with (18) and the result still follows:

$$\lim_{N\to\infty}\left\lfloor \frac{\pi\sqrt{N}}{4}-\frac{1}{2}\right\rfloor\frac{2}{\sqrt{N}}+\frac{1}{\sqrt{N}}=\frac{\pi}{2}. \tag{19}$$

Hence, $\sin^2(p\phi+\phi/2)\to 1$.

With these results, it is then clear that the advantage is at best negligible for large N.

III. PHYSICAL IMPLEMENTATIONS

Here we note that an experimental implementation of the algorithm for the search problem for the three- and four-qubit case is within reach. Recently, there has been an experimental implementation of Grover's algorithm in trapped ions for the three-qubit case [22]. We propose that in such experiments it is possible to implement the variational search algorithm proposed in our work and hence obtain higher probabilities. For such implementations, a gate decomposition for circuits shown in Fig. 4 is needed. The single-qubit gates X, H, R_α, and $\mathrm{C}^k\mathrm{NOT}$ (k-controlled NOT gate with $k=3,4$) are implemented in [22] for the ion trap system. We just need to show how to decompose the k-controlled phase gate such as those shown in Fig. 4. A decomposition is given in [22] that reduces the 3-controlled R_α gate to a pair of Toffoli gates and a 2-controlled R_α, the implementation of which exists experimentally for ions [23].

IV. EFFECT OF NOISE

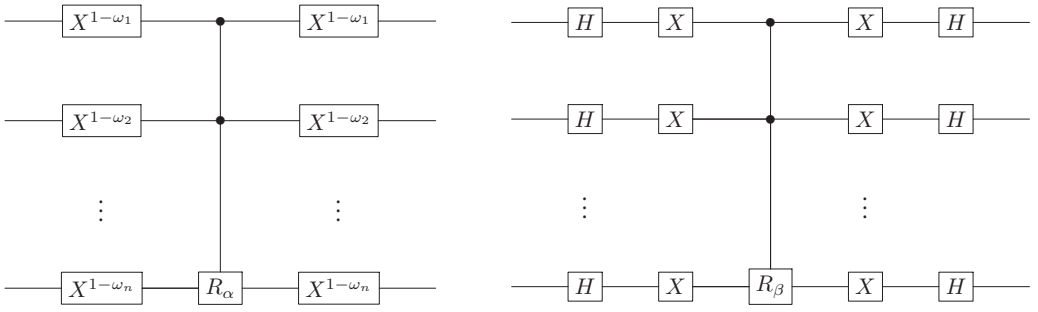
We have also compared both the variational and Grover's algorithm in the presence of noise. For this we have used the Forest SDK [24] and considered T_1 and T_2 noise [25]. This corresponds to so called longitudinal and transversal relaxation times of qubits in the system. The noise is simulated using a Kraus operator approach, yet the Forest SDK works with wave-function simulation, thus several stochastic runs are required. We applied our algorithm using the gate set CZ, $R_z(\theta)$, $R_x(\pm\pi/2)$. The Pyquil library considers one- and two-qubit noise over R_x and CZ, respectively. In Fig. 1 we show the probabilities achieved for the searched string as a function of T_1 and T_2 parameters for the three-qubit search problem. To obtain this plot, the algorithm was run 10 000 times for each T_1 and T_2, and then the probabilities for measuring the searched string were calculated with $T_1, T_2 \in [10^{-6}\ \mathrm{s}, 10^{-2}\ \mathrm{s}]$. The area circled by the red line corresponds to a fit circle inside of which the average difference between the variational algorithm and the optimal probability of Grover's algorithm is greater than 5%. We consider this as a threshold to establish a significant difference even in the presence of noise.

V. DISCUSSION

Let us reflect on several features relating to the most promising results of this study and contrast these with some of the more peculiar shortcomings. An unusual feature of Grover was the small oscillation in the success probability going from unity for two qubits and then decreasing for three and four qubits. This provided some slack for our variational approach to remove. In fact, with one angle (shared by both the oracle as well as the diffusion operator), we do not always match the performance of Grover (for five or more qubits). Additional angles, however, add more degrees of freedom for the optimization procedure to succeed. When considering variational angles for the diffusion operator but not for the oracle operator, there is still the same advantage as in the case of the variational algorithm with only one angle shared between the oracle and the diffusion operator. The advantage disappears when only one variational angle is considered for the diffusion operator, and the standard oracle of Grover's algorithm is used.

We have presented a transfer matrix (11). Interestingly, the optimization procedure is general in the sense that if we restrict to this transfer matrix, this defines the angle(s) for any search item. In other words, if we find the corresponding angle(s) for a given number of items to search in, we can use this same angle again and again for different search items. Nonetheless, it must be noted that the angle(s) obtained through the variational algorithm will only give optimal probabilities for a given number of qubits n in the search problem. For a different n, the algorithm needs to be rerun.

One of the main problems of variational algorithms is how to do classical preprocessing, determine the optimal parameters of an algorithm, and do it efficiently. This paper demonstrates how this procedure can be done for every finite-dimensional search space on a classical computer. It



(a) oracle circuit (b) diffusion circuit

FIG. 4. Circuit realization of diffusion and oracle circuits. Oracle and diffusion operators can be rewritten via n-body control gates $\mathcal{V}(\alpha)=\bigotimes_{i=1}^n X_i^{1-\omega_i}(\mathbb{1}_{2^n-1}\oplus e^{\imath\alpha})\bigotimes_{i=1}^n X_i^{1-\omega_i}$ and $\mathcal{K}(\beta)=H^{\otimes n}X^{\otimes n}(\mathbb{1}_{2^n-1}\oplus e^{\imath\beta})X^{\otimes n}H^{\otimes n}$ and therefore can be realized using $O(n^2)$ basic gates [28]. Here operator $\mathbb{1}_{2^n-1}$ is the $(2^n-1)\times(2^n-1)$ identity matrix. [See also the gate realizations in [22], which can be readily bootstrapped to realize (a) and (b) above.]

means that to find optimal parameters one does not need to vary over a family of quantum circuits during experiment to find an optimal solution. This result looks promising and points out that there is a set of variational quantum problems with parameters that can be efficiently found on a classical computer for an arbitrary number of qubits.

Around the same time as we produced these results, two other teams put out papers that apply machine learning to the optimization and discovery of quantum algorithms [26,27]. These works—appearing just before and then just after ours—are complementary as their approach and the algorithms considered are rather different. In [26] the Swap test algorithm for state overlap is learned using a gate sequencing method similar to ours (but a different gate set). Surprisingly, they find shorter gate depths with the variational algorithm compared to the Swap test. In the case of [27], the authors try a machine learning approach on Simon's algorithm. The optimization method utilized is gradient descent assisted by genetic algorithms by varying over unitaries that depend on a given parameter. They find that this method finds circuits with the same performance as Simon's algorithm. Nonetheless, our work and these two recent papers do share the general concept of training circuits for known algorithms, and the results in these studies illustrate that in the future, quantum algorithm design might be closely tied to the methods presented here.

The source code producing the plots and generating the numerical findings in this study can be found at *Deep Quantum Labs Github* page [29].

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