Deterministic Search on Star Graphs via Quantum Walks

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We propose a novel algorithm for quantum spatial search on a star graph using interleaved continuous-time quantum walks and marking oracle queries. Initializing the system in the star's central vertex, we determine the optimal quantum walk times to reach full overlap with the marked state using $\lceil(\pi/4)\sqrt{N}-(1/2)\rceil$ oracle queries, matching the well-known lower bound of Grover's search. We implement the deterministic search in a database of size seven on photonic quantum hardware, and demonstrate the effective scaling of the approach up to size 115. This is the first experimental demonstration of quantum walk-based search on the highly noise-resistant star graph, which provides new evidence for the applications of quantum walk in quantum algorithms and quantum information processing.

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Introduction.—Searching large databases is an important problem with broad applications. The Grover quantum search algorithm is a hallmark application of quantum computing with a well-known speedup over classical searches of an unsorted database [1–3]. The number of oracle queries required to find a single marked element in an N-element database, approximately $(\pi/4)\sqrt{N}$, is proven to be optimal [4] for large N. The success rate of Grover's algorithm is $1-\mathcal{O}(1/N)$, with subsequent algorithms modifying the state evolution to produce deterministic search [5,6]. In the past two decades, quantum search algorithms have been well investigated theoretically [7–19] and experimentally [20–36].

The "analog analogue" of Grover's algorithm is continuous quantum spatial search on a complete graph $\mathcal{K}_N$ [10,37]. In the Childs and Goldstone ($\mathcal{CG}$) spatial search framework, the system is evolved under a perturbed graph adjacency matrix A with the Hamiltonian $H=-\gamma A-|\omega\rangle\langle\omega|$, where $|\omega\rangle$ is the marked element and γ is a graph-dependent parameter. On the complete graph, when $\gamma=(1/N)$, after evolution time $T=(\pi/2)\sqrt{N}$ the system is rotated from the equal superposition to the marked element. Optimally scaling spatial search is possible on a wide range of other graphs, including the hypercube, lattices of dimension at least four, and almost all large random graphs [19]. Significant recent progress has been made in characterizing the classes of graphs that admit optimal spatial search in the $\mathcal{CG}$ formalism [38]. Spatial search on the star graph, which has been studied in the context of the $\mathcal{CG}$ framework, can be started in the central vertex to achieve 50% overlap with the marked vertex after $\mathcal{O}(\sqrt{N})$ time [39]. The graph Laplacian can also be used in place of the adjacency matrix, resulting in an improved success probability of $1-\mathcal{O}(1/N)$ when initialized in the equal superposition [40]. Additionally, the star graph's simple topology and resistance to noise make it a promising candidate for experimental implementation [40].

In this Letter, we show an optimal and deterministic search on a star graph using a series of alternating phase flips and "diffusion operators," which are continuous-time quantum walks (CTQWs) on an unperturbed star graph. To be explicit, our algorithm has 100% theoretical success probability for any database size N. Since simulation of QW on a star graph can be fast forwarded [41], this results in an efficient gate model search algorithm. We show the query complexity of deterministic quantum search on the star graph structure matches Grover's algorithm for unsorted databases. Additionally, our algorithm only uses marked vertex phase flips, rather than the generalized phase rotations that are more costly but typically used for deterministic search [5,6]. This leads to a significantly more efficient deterministic search circuit.

We investigate the stability and performance of the algorithm experimentally, using single photons and linear optical elements. This is the first physical demonstration of quantum walk-based search on a star graph. We demonstrate searching a database of size seven as an example, and show that using the theoretically deterministic algorithm gives high probability of success in practice, even after multiple iterations. This work naturally raises questions about speed-up in star graphs, which can now be investigated by using our method and such a single-photon interferometric network. Our work opens up an avenue of applications of quantum information for real-world search-based tasks on near-term quantum hardware, with the spatial graph chosen to suit the quantum hardware.

Theoretical idea.—The generalized Grover state evolution is expressed as

$$|\vec{\alpha},\vec{\beta}\rangle = \left(\prod_{i=1}^{p} U_s(\beta_i)U_f(\alpha_i)\right)|\psi\rangle, \tag{1}$$

where $U_f(\alpha) = \mathbb{1} + (-1 + e^{i\alpha})|\omega\rangle\langle\omega|$ applies a controlled phase rotation to the marked element(s), and $U_s(\beta) = \mathbb{1} + (-1 + e^{i\beta})|\psi\rangle\langle\psi|$ is a generalized reflection about the equal superposition $|\psi\rangle$. When $\alpha = \beta = \pi$, standard Grover search is obtained. For other values of $\vec{\alpha}$ and $\vec{\beta}$, one can achieve deterministic search [5,6] or optimal fixed-point search [42].

In this Letter, we consider a further important generalization of the Grover state evolution for spatial quantum search, wherein the generalized reflection about the equal superposition $U_s(\beta)$ is replaced by a CTQW $U_w(t) = e^{-iAt}$ on an undirected graph with adjacency matrix A [43,44]. Specifically, in this work we focus on a CTQW for a star graph $U_w(t) = e^{-itS_N}$, where

$$S_N = \sum_{x\neq c}(|c\rangle\langle x| + |x\rangle\langle c|) \tag{2}$$

with a central vertex $|c\rangle$ connected to N outer vertices $|x\rangle$. A star graph with eight total vertices is shown in Fig. 1(a), where here the central vertex is encoded as $|c\rangle = |0\rangle$ and the marked vertex is $|7\rangle$.

The walking operator, as the time evolution of the adjacency matrix S_N, has action

$$U_w(t)|c\rangle = \cos\sqrt{N}t|c\rangle - \frac{i\sin\sqrt{N}t}{\sqrt{N}}\sum_{x\neq c}|x\rangle,$$

$$U_w(t)|x\rangle = |x\rangle + \frac{-1+\cos\sqrt{N}t}{N}\sum_{y\neq c}|y\rangle - \frac{i\sin\sqrt{N}t}{\sqrt{N}}|c\rangle. \tag{3}$$

To achieve search with certainty, we use the state evolution $-i|\omega\rangle = (\prod_{i=1}^{p} U_w[(-1)^i t_{N,p}]U_f(\pi))|s\rangle$, where $|s\rangle = U_w(t_{N,p}/2)|c\rangle$ is the initial state, and $t_{N,p} = (2/\sqrt{N})\arcsin\{\sqrt{N}\sin[\pi/2(1+2p)]\}$. That is, starting in the central vertex $|c\rangle$, the initial state is constructed with a first QW. Then a series of marked vertex phase flips

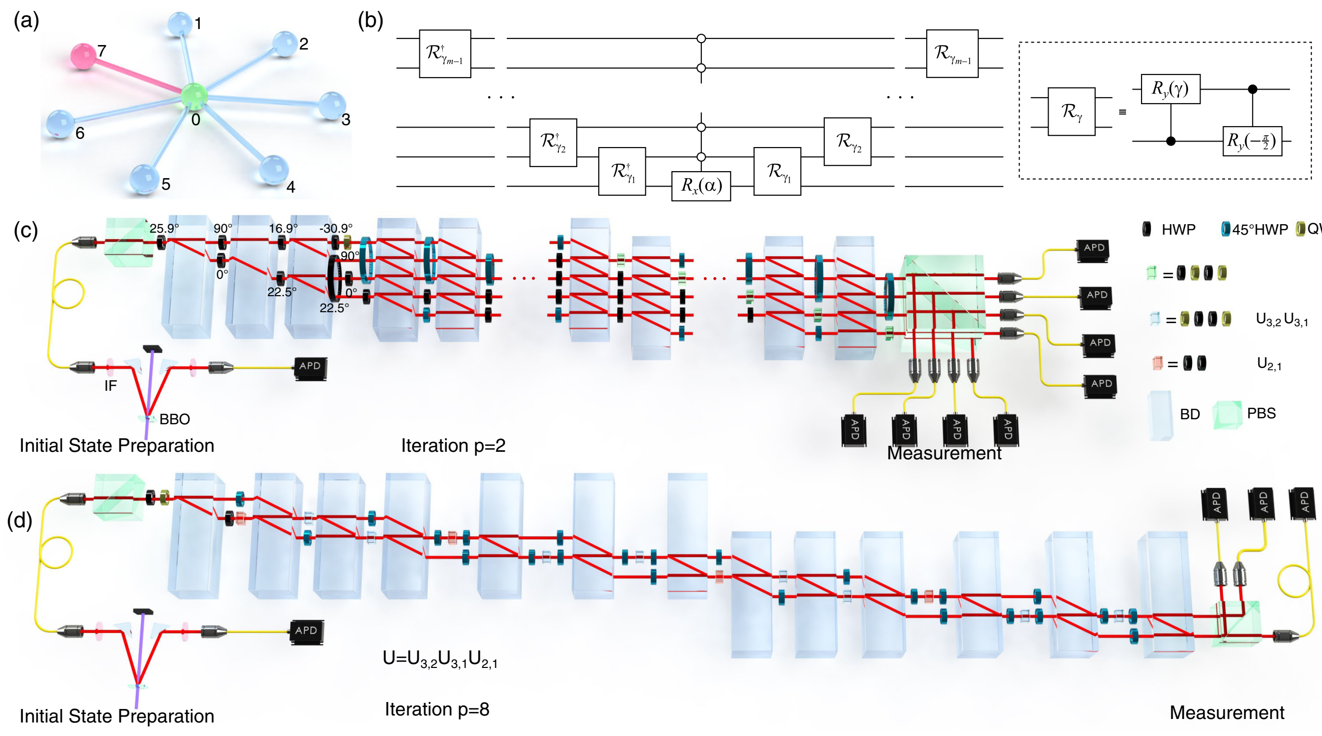

FIG. 1. (a) A star graph S_7, consisting of seven outer vertices connected to a central vertex. (b) Efficient quantum circuit to simulate a CTQW over the star graph S_N where $N+1 = 2^m$, without ancillas. Here, $\gamma_k = 2\arccos(2^{m-k+1}-1)^{-1/2}$ and $\alpha = -2\sqrt{N}t$. (c),(d) Experimental setup. A pair of photons is generated via the spontaneous parametric down-conversion, with one serving as a trigger and the other as a single photon. (c) For a higher-dimensional system, quantum states are encoded in both polarizing and spatial degrees of freedom and prepared by beam displacers (BDs, $22.5\times10\times28.3$ mm) followed by a polarizing beam splitter (PBS) and wave plates (WPs). It then undergoes an optical network which implements an evolution of searching, composed of WPs and BDs, and finally is projected into the basis states via a PBS. Finally the signal photon is detected by avalanche photodiodes, in coincidence with the trigger photon, having a coincident window of 3 ns. (d) Setup for the Grover search algorithm in the 3×3 subspace. We use eight iterations of evolution as an example.

and QWs are applied, reaching full overlap with the marked vertex $|\omega\rangle$ after p iterations. In order to make the walk times real valued, the requirement on p is

$$p \geq \left\lceil \frac{\pi}{4}\sqrt{N} - \frac{1}{2} \right\rceil. \quad (4)$$

We assume without loss of generality that $|c\rangle \neq |\omega\rangle$, by performing a preliminary oracle query on the central vertex.

Quantum circuit and oracle queries.—We provide an efficient quantum circuit for fast-forwarded CTQWs on the star graph S_N for $N = 2^m - 1$ in Fig. 1(b), improving upon the approach for simulation based on general bipartite graphs given in [41] by reducing the number of qubits required. This circuit treats $|c\rangle = |0\rangle$ in the computational basis, with $|x\rangle$ for $x = 1, \ldots, N$ labeling the outer star vertices. The circuit can be decomposed into $\mathcal{O}(\log N)$ one- and two-qubit gates using a single ancilla, or $\mathcal{O}(\log^2 N)$ with no ancilla qubits [45]. Details of the circuit's correctness can be found in Supplemental Material [46].

The other component is the controlled phase flip operator, which applies a negative phase to the marked vertex. We address the advantage of exclusively using $U_f(\pi)$, rather than the generalized phase rotation $U_f(\theta)$. Suppose one has access to a conventional quantum black box

$$\mathcal{A}|x\rangle|y\rangle = |x\rangle|y \oplus (x = \omega)\rangle, \quad (5)$$

that flips the ancilla qubit iff $|x\rangle$ is marked. Then to produce the phase-flip oracle utilized in quantum search, phase kickback is utilized: here the ancilla qubit is set to $|-\rangle = (1/\sqrt{2})(|0\rangle - |1\rangle)$ so that $\mathcal{A}|x\rangle|-\rangle = (-1)^{x=\omega}|x\rangle|-\rangle = (U_f(\pi)|x\rangle)|-\rangle$. However, this trick is only applicable when a phase flip is required, rather than the more general phase rotation given in Eq. (1). The general case necessitates an application of $\mathcal{A}^\dagger$ as well to perform uncomputation, thus, in essence, doubling the number of "fundamental" oracle queries. A circuit for this general case is provided in [42]. Thus, it is beneficial in practice, where possible, to restrict search algorithms to usages of $U_f(\pi)$. The star graph search algorithm described in this Letter meets this criteria, making it an excellent approach to deterministic database searching.

Experimental implementation.—We demonstrate the deterministic searching by simulating CTQWs on a S_7 star graph using single photons and linear optics as illustrated in Fig. 1(c). We construct the 8×8 unitary operator for S_7, which has one central node and seven outer nodes, and simulate the time evolution. In this experiment, the basis states of an eight-dimensional qudit are encoded as $|0\rangle = |H1\rangle, |1\rangle = |V1\rangle, |2\rangle = |H2\rangle \ldots |7\rangle = |V4\rangle$, where $|i\rangle$ $(i = 1, \ldots, 4)$ represents the spatial modes of the single photons, $|H\rangle$ and $|V\rangle$ represent the horizontal and vertical polarizations of the photons [47–51]. The state of the central vertex is $|c\rangle = |0\rangle$ and for this demonstration the marked vertex is chosen to be $|\omega\rangle = |7\rangle$.

In our experiment, the initial state of the qudit is prepared in $|s\rangle = 0.576i|0\rangle + 0.309\sum_{j=1}^{7}|j\rangle$. First, after passing through a polarizing beam splitter (PBS) and a half-wave plate (HWP) at 25.9°, the transmitted photons with the polarization $0.618|H\rangle + 0.786|V\rangle$ are split into two parallel paths by a beam displacer (BD). Second, two HWPs at 90° and 0 are inserted into the upper and lower modes, respectively. Similarly, after going through the second BD, two HWPs at 16.9° and 22.5° are inserted into the upper and lower modes, respectively. Finally, after the third BD followed by three HWPs (at −30.9°, 22.5°, and 0, respectively) and a quarter-wave plate at 90°, the state is prepared in $|s\rangle$.

In order to implement a search on the star graph with eight vertices, we need to construct a 8×8 walking operator U_w and a marking oracle $U_f(\pi)$. The optimal walk time is $t_k = (-1)^k \times 0.724$ $(k = 1, 2)$ and the optimal number of iterations is $p = 2$. Thus, we apply the unitary operation $U = U_w(0.724)U_f(\pi)U_w(-0.724)U_f(\pi)$ on the state $|s\rangle$ and the final state then has 100% overlap with the marked state. In the basis $\{|i\rangle\}$, the 8×8 unitary operator U can be decomposed into [52]

$$U = U_{8,7} \cdots U_{8,1} U_{7,6} \cdots U_{7,1} \cdots U_{2,1}. \quad (6)$$

Each U_{ij} is an 8×8 transformation acting only on a two-dimensional subspace of the eight-dimensional Hilbert space with the complementary subspace unchanged. Only four elements E_{ii}, E_{ij}, E_{ij} and E_{jj}, are neither 0 or 1. All the other diagonal elements are 1 and all the off-diagonal elements are 0. To realize U_{ij}, we combine two different spatial modes into one via BDs and WPs and then apply a 2×2 transformation $\left(\begin{smallmatrix} E_{ii} & E_{ij} \\ E_{ji} & E_{jj} \end{smallmatrix}\right)$ on the polarizations of photons in this mode, as an arbitrary 2×2 transformation of the polarization of a photon can be realized via a set of WPs.

The overlap between the final state and the marked state is obtained by a two-qubit projective measurement. A PBS is used to perform the projective measurement on the photons in the basis $\{|i\rangle\}$. The clicks of the detectors correspond to the probabilities of the final state projected onto the basis states. From the probability distribution of the basis states we can calculate the overlap between the final state and the marked state as the squared root of the probability of the final state being found in $|7\rangle$.

Figure 2 shows the results of the star search algorithm on S_7 by comparing theoretical predictions and experimental results of the overlap between the final state and the marked state for the first 12 search iterations. The overlaps after the second, seventh, and twelfth iterations are 0.891 ± 0.002, 0.906 ± 0.002, and 0.899 ± 0.002, respectively, which agree well with the theoretical prediction of 1. As $U^5 = \mathbb{1}$, the evolution is essentially periodic with a period $T = 5$ as shown in Fig. 3(a). Thus, using a modified initial state,

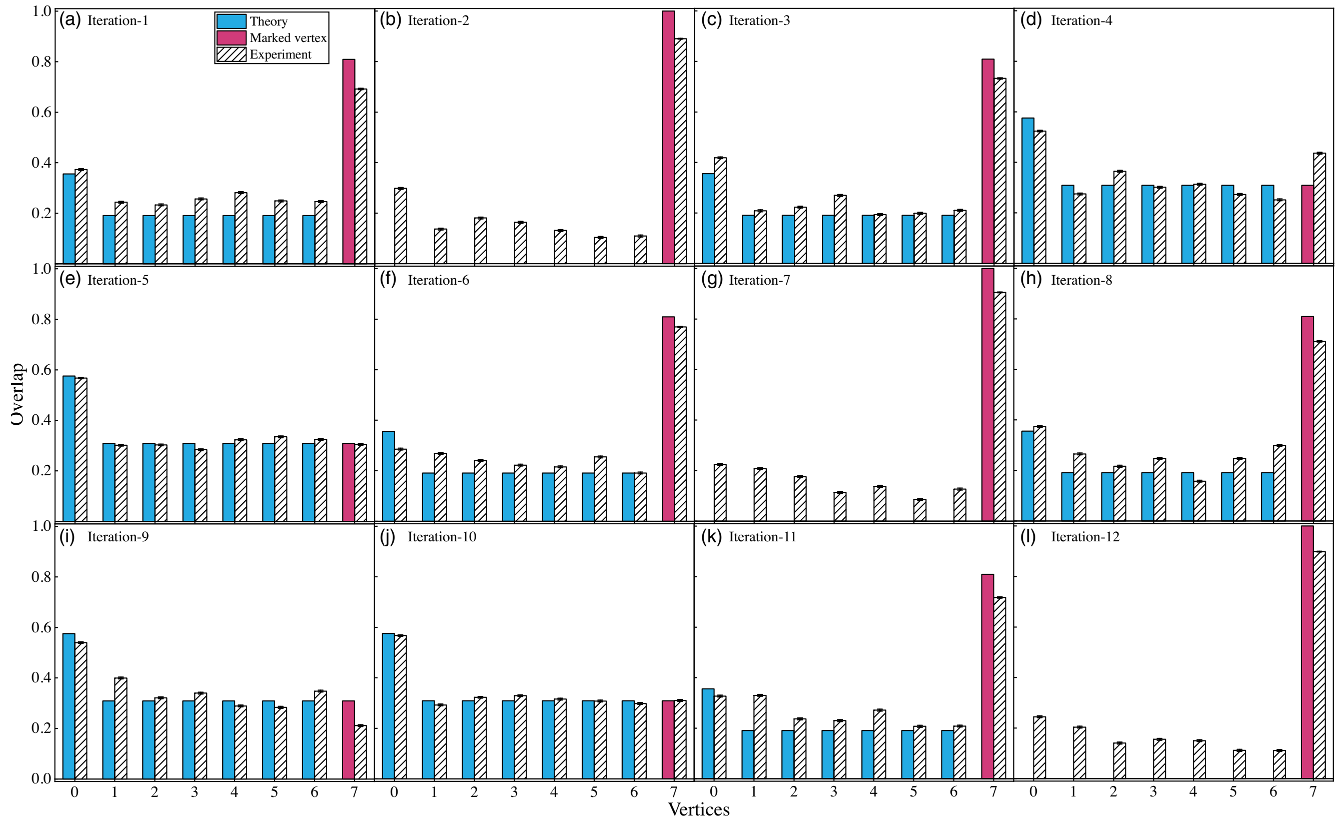

FIG. 2. Experimental results of the star search algorithm in a database of size seven by comparing theoretical predictions and experimental results of the overlap between the final state and the marked state for the first 12 iterations of searching. Error bar indicates the statistical uncertainty which is obtained based on assuming Poissonian statistics.

we find for $N = 7$ the search algorithm reaches full overlap with the marked state in $2 + 5x$ iterations, where x is a positive integer.

One can also perform a quantum simulation of the searching process by direct implementation of the algorithm in the three-dimensional subspace $\{|c\rangle, |\omega_\perp\rangle, |\omega\rangle\}$, where $|\omega_\perp\rangle$ is the equal superposition over the unmarked outer vertices. This assumes prior knowledge of the marked vertex. The quantum simulation of the search is useful to study the coherence of the quantum system after multiple iterations. A quantum simulation of the searching process by direct implementation of the algorithm in the three-dimensional subspace can be realized with a similar setup and the number of the BDs n increases with the number of iterations p linearly, i.e., $n \sim 3p/2$. The setup for the quantum simulation can be further simplified and can always be realized with 3 BDs, as the number of iterations can be regarded as a parameter of the transformation operation and tuned by the setting angles of WPs.

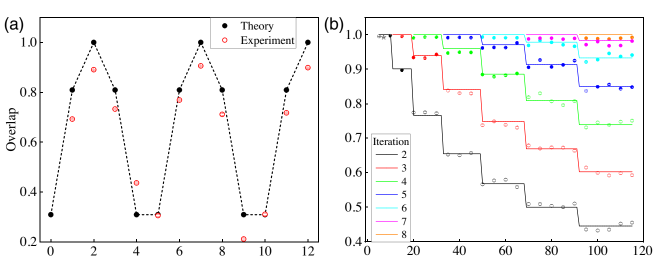

FIG. 3. (a) Overlaps between the final state and the marked state versus the number of iterations for 12 iterations of searching in an eight-vertex star graph. (b) Experimental results of the Grover search algorithm in the subspace with the database of size from 5 to 115 by comparing theoretical predictions and experimental results of the overlap between the final state and the marked state.

To demonstrate the dynamics in the subspace, the basis states are encoded as $|0\rangle = |V1\rangle$, $|1\rangle = |H2\rangle$, and $|2\rangle = |V2\rangle$. The state of the central vertex is $|0\rangle$ and that of the marked vertex is $|2\rangle$. For each N, we can determine the marking oracle, the CTQW times, the initial state $|s\rangle$, and the optimal number of iterations for a deterministic search as per Eq. (4).

In our experiment in Fig. 1(d), the initial qutrit state in the subspace is generated via a PBS, a BD, and WPs. As we mention above, our experimental setup with linear optics can implement an arbitrary unitary operation. For each iteration, the 3×3 operation can be decomposed and implemented via two BDs and WPs. We choose database sizes $N = 5, 10, \ldots, 115$ to prove the validity of our optimal and deterministic spatial search algorithm. Figure 3(b) shows the results of the Grover search algorithm in the database of sizes 5–115 by comparing theoretical predictions and experimental results of the overlap between the final state and the marked state. The optimal number of iterations for search increases proportionally to the square root of the size of the database. For size $N = 115$, we need $p = 8$ iterations to reach 100% overlap. Experimentally, the overlap is 0.9920 ± 0.0005 which agrees with theoretical prediction very well. To compare the search in the subspace to that of the original Hilbert space, we also study the $N = 7$ case. As expected, search in the subspace is achieved after two iterations and the overlap between the final state and the marked state is 0.9921 ± 0.0005.

Discussion and conclusion.—In this Letter, we have investigated the star graph under a spatial search framework that applies alternating controlled phase shifts and CTQWs. The algorithm can be initialized in the central vertex and exactly produces the marked vertex state $-i|\omega\rangle$ in $\lceil (\pi/4)\sqrt{N} - \frac{1}{2} \rceil$ iterations. Compared to the conventional approach for spatial search [10], our approach is more flexible and is directly implementable on gate model hardware without the need for Trotterization. Since CTQWs on the star graph can be fast-forwarded, this results in an efficient gate model circuit for deterministic search, by replacing the Grover diffusion operator with the walking circuit and modifying the initial state. The simple topology of the star graph has advantages for physical hardware [40].

Our work is the first experimental demonstration of this new and more flexible database search framework, as well as the first experimental demonstration of deterministic spatial search. In doing so we show the advantages of selecting a graph to suit the quantum hardware. This work thus demonstrates the alternating phase-walk framework's advantages on near-term quantum hardware in reducing the impacts of noise, on the widely applicable problem of searching a database.

We implement the star search technique using photonics, where the experimental results show high agreement with the theory. The state evolution results are studied for a specific eight-vertex example, and additionally in the walk subspace for star graphs with up to 116 vertices. In fact, the setup is sustainable for application to comparably large databases. For size N, the number of the bulk optical elements (BDs) n increases with N linearly, i.e., $n \sim 2(N+1) - 4$.

The implementation setup, consisting of a series of alternating applications of controlled phase shifts and QWs, has been shown to be applicable to any graph having rational eigenvalues, with the appropriate walk times determinable in closed form [43]. Deterministic and efficient quantum search using this framework has also been shown on a class of interdependent network graphs [44] and also has strong ties to perfect state transfer [53,54]. A topic of future study is to fully characterize the class of graphs that permit deterministic search, with practical applications for improving success probability in practice on near-term intermediate-scale quantum hardware having connectivity constraints [55].

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