Controlled quantum search on structured databases

Yunkai Wang,[1,2] Shengjun Wu,[1,3,*] and Wei Wang[3,†]

[1]*Institute for Brain Sciences and Kuang Yaming Honors School, Nanjing University, Nanjing 210023, China*

[2]*Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA*

[3]*National Lab of Solid State Microstructure, Collaborative Innovation Center of Advanced Microstructures, and Department of Physics, Nanjing University, Nanjing 210093, China*

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By proposing two schemes (namely, a multistage and a single-stage one) based on the continuous-time quantum walk (CTQW), we study the quantum search on balanced trees of height r with N vertices. For the multistage scheme, we achieve the search for a marked leaf vertex with a runtime $\Theta(N^{(2r-1)/2r})$ and a success probability close to 100% when the branching factor is large. For the single-stage scheme with adjustable edge weights, we achieve the search with an optimal runtime $\Theta(\sqrt{N})$ and a success probability close to 100% as well. Furthermore, we show that our search algorithms also work for real trees with unbalanced structures and are quite robust against various kinds of small perturbations.

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I. INTRODUCTION

In the Yellow Pages, each entry contains a subscriber's name, phone number, and other information. All the entries are ordered alphabetically according to the subscribers' names, and the whole directory can be considered as a structured tree with each entry corresponding to a vertex (see Fig. 1). One can easily find the phone number of a subscriber since the path to the related entry is directly following the name. Nevertheless, it is very difficult to find the related subscriber's name when only his/her phone number is given since one does not know the path to the corresponding entry. Thus the search on this database requires an average runtime proportional to the total number of the phone entries N and is actually equivalent to that on an unsorted database. For such an unsorted database, if the vertices are mimicked to certain kind of quantum counterparts, interestingly, a fast quantum search via the Grover's algorithm [1] can be applied, providing a quadratic quantum speedup with a runtime $\Theta(\sqrt{N})$. Although the implementation of the Grover's algorithm is not easy, it was shown that on complete graphs a standard continuous-time quantum walk (CTQW) can realize the continuous-time analog of the Grover's algorithm and achieve a quadratic quantum speedup [2]. Generally, for many databases, e.g., the phone directories, with tree structures, one may still expect that a search via the standard CTQW can achieve the same quantum speedup, but a study showed that the standard CTQW on trees cannot achieve the mentioned above quantum advantage [3]. Can we use a generalized scheme based on modified CTQW to realize the quantum search on databases with tree structures and achieve the quantum speedup?

The model of quantum walk describes a particle evolving on a graph according to a unitary evolution operator determined by the structure of the graph [4,5]. This model is quite friendly for algorithmic design and experimental implementation [6,7]. It has already been used as an algorithmic tool to design the quantum algorithms [8–10], implement the universal quantum computing [11–13], explore the topological insulator and photonics [14,15], generate the nonclassical states in optics [16], model the network-based process [17], study the properties related to localization [18,19], and even test some aspects of the fundamental physics [20,21]. Its experimental implementations or proposals were explored in different platforms: trapped ions and atoms [22–25], optical systems [21,26–29], nuclear-magnetic-resonance devices [30], quantum circuits [31], and the artificial electric field [32]. In addition, except the complete graphs, algorithms based on CTQW was also used to the spatial search on the hypercube, d-dimensional periodic lattices [2], and several other graphs [3,33–39]. An optimal search time $\Theta(\sqrt{N})$ was obtained for some of these structured graphs under certain circumstances [2,34–37]. However, it was also shown that high connectivity, good global symmetry and regularity do not guarantee fast search [36–38].

Tree structures are very important and essential for data manipulation. Organizing quantum memory in tree-structure has gotten some attention as it allows a easy way for addressing [40–42]. There have been a number of ingenious studies on quantum algorithm related to trees [3,5,8,34,43–50]. As a typical example, the search for a hidden tree vertex was achieved via the CTQW within a runtime $\Theta(N^{\beta})$ with β varying from 0.5 to 1 when the marked vertex moves from the root (the single vertex on the top level) to the leaves (the vertices in the bottom level with no children) [3]. Thus no

*sjwu@nju.edu.cn
†wangwei@nju.edu.cn

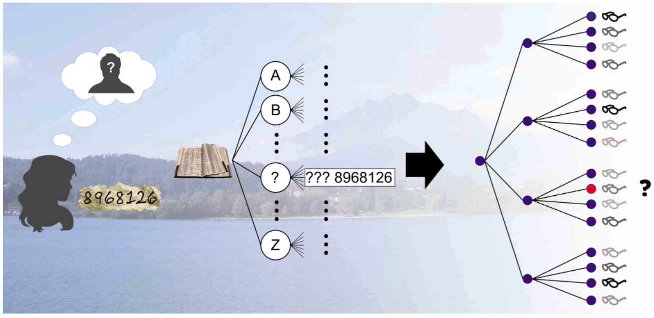

FIG. 1. A physicist's conundrum. Having a ragged note with a phone number on it, a physicist tries to find out the owner out of curiosity. Can a quantum walk help her to find this particular phone entry?

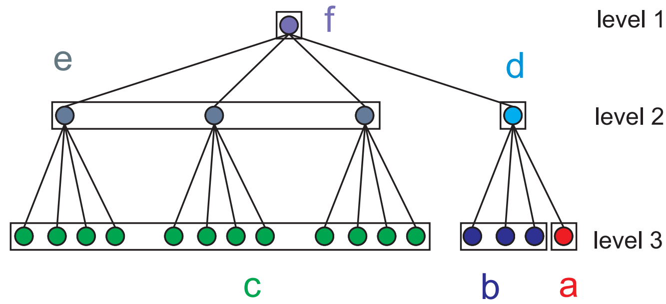

FIG. 2. A balanced tree with height $r = 2$ and branching factor $M = 4$. The total number of vertices is $N = 1 + M + M^2 = 21$. The invariable subspace is spanned by the six states $|a\rangle, \cdots, |f\rangle$, with each one an equal superposition of the vertex states in the corresponding box.

quantum speedup is obtained when the vertex is deeply hidden as a leaf. Moreover, the success probability is rather low, and practically decreases as the height of the tree increases. In another work, the success probability was shown to be much less than 100%, and also decreases as the height or branching factor increases [34] (see Sec. II D of Ref. [51] for more discussions). In a nice recent work via the discrete-time quantum walk [50], the structure of the graph is modified according to the result of each trial and a speed close to (still slower than) the Grover's algorithm is achieved, but this approach requires multiple trials. It is still a challenge to have an optimal runtime and a high success probability at the same time for the search on a tree.

In this paper, we provide a solution. We propose a multistage quantum search scheme on trees with a success probability close to 100%, which does not decrease as the height or branching factor of the tree increases. Surprisingly, we also find that a proper modification of the edge weights can cause a merging of the multistages in the search processes, thus resulting in a substantial speedup for the search. With a suitable choice of the edge weights, we can achieve an optimal runtime $\Theta(\sqrt{N})$, meanwhile keep the high success probability.

II. GENERAL SCENARIO

We consider a particle that performs a quantum walk on a graph with N vertices, with each vertex corresponding to a basis state in an N-dimensional Hilbert space. The quantum walk is governed by the Hamiltonian [2]

$$H = -\gamma L - |a\rangle\langle a|, \tag{1}$$

where γ is the jumping rate (amplitude per unit time) between a pair of connected vertices, $L = A - D$ is the graph Laplacian, A is the adjacency matrix of graph (i.e., A_{ij} is the weight of edge between vertices i and j), D is the diagonal matrix with $D_{jj} = \deg(j)$ (i.e., the total weight of edges connected to vertex j), and $|a\rangle$ is the state corresponding to the marked vertex a. For convenience, our Hamiltonian H and the time are chosen to be dimensionless. Quantum algorithms usually use an invariant subspace of the Hamiltonian, which can be conveniently found by grouping the identically evolving vertices together. Since we have no prior information of the location of the marked vertex, the initial state of the particle is chosen as

$$|s\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} |i\rangle. \tag{2}$$

The quantum search proceeds as follows. We start with the initial state $|s\rangle$ in Eq. (2) in the invariant subspace, and let the particle evolve under the Hamiltonian in Eq. (1). After a particular period of time, the particle will arrive at the marked vertex a with a certain probability. We then perform a projective measurement onto the vertex basis and reveal the marked vertex with a probability P of success. If the jumping rate is fixed and the edge weights are uniformed, the success probability P is low and decreases when the height or the branching factor increases in general. Here we take the advantage of controllable jumping rate and adjustable edge weights to improve the success probability and search speed.

III. MULTISTAGE QUANTUM SEARCH ON BALANCED TREES

We focus on a balanced tree with height r and branching factor M, which contains one vertex on the first (top) level, M vertices on the second level, ..., and M^r vertices on the $(r+1)$th (bottom) level, thus the total number of $(M^{r+1} - 1)/(M - 1)$ vertices (see Fig. 2). We assume that the marked vertex is a leaf vertex.

We first discuss a balanced tree with height $r = 2$ and an arbitrary branching factor M (see Fig. 2 for the case of $M = 4$). To study the evolution of the system, we group the vertices with identical evolution by the same color, and then work in the invariant subspace of the Hamiltonian. The invariant subspace is spanned by the following six basis states: $|a\rangle$ (the marked vertex state), $|b\rangle = \frac{1}{\sqrt{M-1}} \sum_{i\in b} |i\rangle$, $|c\rangle = \frac{1}{\sqrt{M(M-1)}} \sum_{i\in c} |i\rangle$, $|d\rangle$, $|e\rangle = \frac{1}{\sqrt{M-1}} \sum_{i\in e} |i\rangle$, and $|f\rangle$. A state initially in the invariant subspace evolves only in the subspace due to the vanishing off-diagonal terms of the Hamiltonian between the invariant subspace and its orthogonal complement.

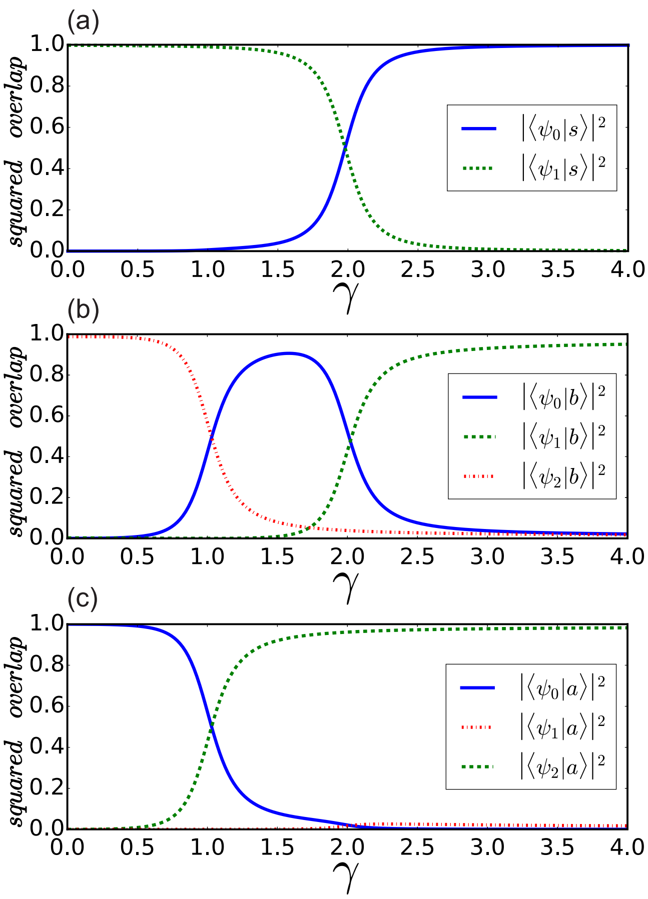

FIG. 3. The squared overlaps of basis states $|s\rangle$, $|b\rangle$, $|a\rangle$ with the eigenstates $|\psi_{0,1,2}\rangle$ of H for a balanced tree of height 2 when $M = 100$.

Hence, the effective Hamiltonian in this subspace is

$$H = -\gamma \begin{bmatrix} -1+\frac{1}{\gamma} & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & \sqrt{M-1} & 0 & 0 \\ 0 & 0 & -1 & 0 & \sqrt{M} & 0 \\ 1 & \sqrt{M-1} & 0 & -M-1 & 0 & 1 \\ 0 & 0 & \sqrt{M} & 0 & -M-1 & \sqrt{M-1} \\ 0 & 0 & 0 & 1 & \sqrt{M-1} & -M \end{bmatrix}.$$

The evolution of the particle's state is determined by a Schrödinger's equation with solution

$$|\psi(t)\rangle = e^{-iHt}|s\rangle = e^{-iHt}\sum_{i=0}^{5}|\psi_i\rangle\langle\psi_i|s\rangle, \tag{3}$$

where $|\psi_i\rangle$ is the ith lowest eigenstate of H and can be worked out numerically. The overlaps between the basis states and the eigenstates of H as functions of γ are shown by Fig. 3. From it we know that the first two eigenstates $|\psi_i\rangle(i = 0, 1)$ of H are equal superpositions of $|b\rangle$ and $|s\rangle$ when $\gamma = 2$, and direct numerical calculations yield $|\psi_0\rangle \approx (|b\rangle + |s\rangle)/\sqrt{2}$ and $|\psi_1\rangle \approx (|b\rangle - |s\rangle)/\sqrt{2}$ (the approximation becomes more accurate when M increases and the deviation as function of M is shown by Fig. S2 in Ref. [51]). We have

$$|\psi(t)\rangle = e^{-iHt}|s\rangle \approx \frac{1}{\sqrt{2}}(e^{-iE_0t}|\psi_0\rangle + e^{-iE_1t}|\psi_1\rangle), \tag{4}$$

and then $|\langle b||\psi(t)\rangle|^2 = (1 - \cos\Delta E_{10}t)/2$, where $\Delta E_{10} = E_1 - E_0$. Hence, the probability amplitude will flow from $|s\rangle$ ($\approx|c\rangle$) to $|b\rangle$ within a time $\pi/\Delta E_{10}$. Similarly, when $\gamma = 1$, the state of the system oscillates between $|b\rangle$ and $|a\rangle$. In order to make the probability amplitude accumulate in the marked vertex a, a two-stage process is required and works as follows. In the first stage, the system is prepared in the initial state $|s\rangle$, and evolves according to the Hamiltonian with $\gamma = 2$ during a time $\pi/\Delta E_{10}$. Then, in the second stage, the system evolves according to the Hamiltonian with adjusted jumping rate $\gamma = 1$ for a time $\pi/\Delta E_{20}$. Finally, a simple projective measurement onto the vertex states will reveal the state $|a\rangle$ for the marked vertex a with a very high probability. The evolution of probability distribution illustrated in Fig. 4 clearly shows the state evolution $|s\rangle(\approx|c\rangle) \to |b\rangle \to |a\rangle$ step by step (and also see Fig. S5 in Sec. II B of Ref. [51] for a pictorial demonstration).

For the first stage with $\gamma = 2$, by numerically calculating the slope of $\ln(E_1 - E_0)$ as a function of $\ln M$ as shown in Fig. 5 (details in Sec. II A of Ref. [51]), we find the energy gap

$$\Delta E_{10} = 4.0M^{-3/2} - 10M^{-5/2} + o(M^{-5/2}). \tag{5}$$

Considering only the dominant term, we obtain the searching time in the first stage as

$$t = \pi M^{3/2}/4. \tag{6}$$

For the second stage with $\gamma = 1$, we find

$$\Delta E_{20} = 2.0M^{-1/2} - 1.75M^{-3/2} + o(M^{-3/2}), \tag{7}$$

and we obtain the searching time in this stage as

$$t = \pi M^{1/2}/2. \tag{8}$$

When M is large enough, e.g., $M = 100$, the success probability $|\langle a||\psi(t)\rangle|^2$ for finding the marked vertex in the final projective measurement is close to 100%, indicating all higher order terms dropped are negligible. The effect of M on the success probability P is shown in Sec. II C of Ref. [51], where a discussion on the effect of higher order terms dropped here is also given. The dominant term of the runtime in the overall search process is $t \propto M^{3/2} \propto N^{3/4}$.

Now, we discuss the case of any height r. We explicitly write down the Hamiltonian in the invariant subspace and work out the related results for r up to 6. We find that the search process with a high success probability has r stages with different jumping rates $\gamma = r, r-1, \ldots, 2, 1$, and the appropriate searching time in each stage is proportional to $M^{1/2}, M^{3/2}, \ldots, M^{(2r-3)/2}$, and $M^{(2r-1)/2}$ (i.e., $N^{1/2r}, N^{3/2r}, \ldots, N^{(2r-3)/2r}$, and $N^{(2r-1)/2r}$), respectively. The dominant term of the time required in the search process is $\propto M^{(2r-1)/2} \propto N^{(2r-1)/2r}$.

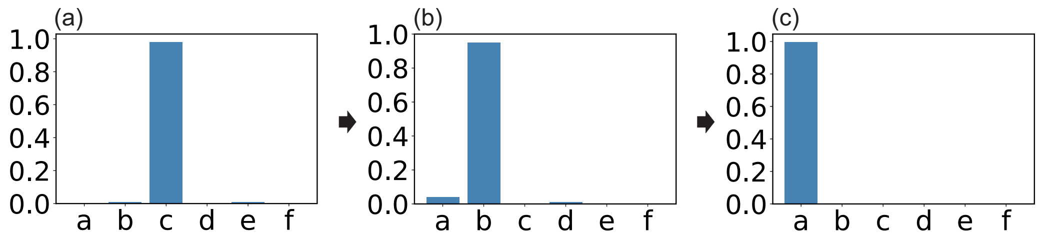

FIG. 4. The evolution of probability distribution for a balanced tree with $r = 2$ and $M = 100$. The probability distribution is illustrated for the state at the beginning (a), at the end of the 1st step (b), and at the end of the second step (c). At the end of the second step (c), the probability in the marked state $|a\rangle$ is close to 100%.

IV. MERGED SINGLE-STAGE QUANTUM SEARCH

A. The goal

Our multistage quantum search on balanced trees achieves a high success probability with a runtime $\Theta(N^{(2r-1)/2r})$. Can we further improve the search scheme to achieve an optimal runtime $\Theta(N^{1/2})$ while keeping the high success probability? A positive and even surprising answer is given below. By adjusting the edge weights, we can merge our multistage search process into a single stage and achieve an optimal search speed with runtime $\Theta(N^{1/2})$!

B. The case with height $r = 2$

Let us start with a balanced tree with height 2. We adjust the weight of edges between the first and second level and set it as ω. The invariant subspace is the same as before, and the effective Hamiltonian in the invariant subspace is written as

$$H = -\gamma \begin{bmatrix} -1+\frac{1}{\gamma} & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & \sqrt{M-1} & 0 & 0 \\ 0 & 0 & -1 & 0 & \sqrt{M} & 0 \\ 1 & \sqrt{M-1} & 0 & -M-\omega & 0 & \omega \\ 0 & 0 & \sqrt{M} & 0 & -M-\omega & \omega\sqrt{M-1} \\ 0 & 0 & 0 & \omega & \omega\sqrt{M-1} & -\omega M \end{bmatrix}.$$

For a given value of ω, the search with high success probability is a two-stage process with two different jumping rates in general. However, we observe that when the value of ω increases from $O(M^{1/4})$ to roughly $O(M^{3/4})$, the two stages in the search process are merged gradually, and then become a single stage for the value of $\omega > O(M^{3/4})$. Enlightened by this observation, we consider a single-stage process and assume $\omega = M$ in the following. Figure 6 shows the squared overlaps between the basis states and the eigenstates of H (more details in Sec. III A of Ref. [51]). When $\gamma = 1 + 1/M$, we find that

$$E_1 - E_0 = 2M^{-1} - 2M^{-2} + o(M^{-2}), \tag{9}$$

and we obtain the searching time as

$$t = \pi M/2 \propto N^{1/2}. \tag{10}$$

Compared to the original two-stage search process, which gives a runtime $t \propto M^{3/2} \propto N^{3/4}$, a substantial speedup is achieved for the weighted graph. We also find that the success probability P is close to 100% when M is large enough. The influence of M on the success probability P is shown in Fig. S9 (Sec. IIIB of Ref. [51]). We have obtained similar results for a balanced tree with height 3 (Sec. IIIC of Ref. [51]). The runtime $t \propto N^{5/6}$ in a three-stage search is shortened to an optimal runtime $t \propto N^{1/2}$ in the single-stage search with adjusted weights.

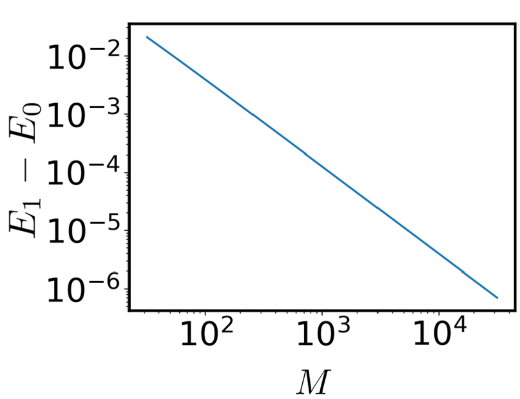

FIG. 5. The relation between energy gap $E_1 - E_0$ of the balanced tree of height 2 and the branching number M. The slope of the line in the figure shows that the energy gap $E_1 - E_0$ scales as $M^{-3/2}$.

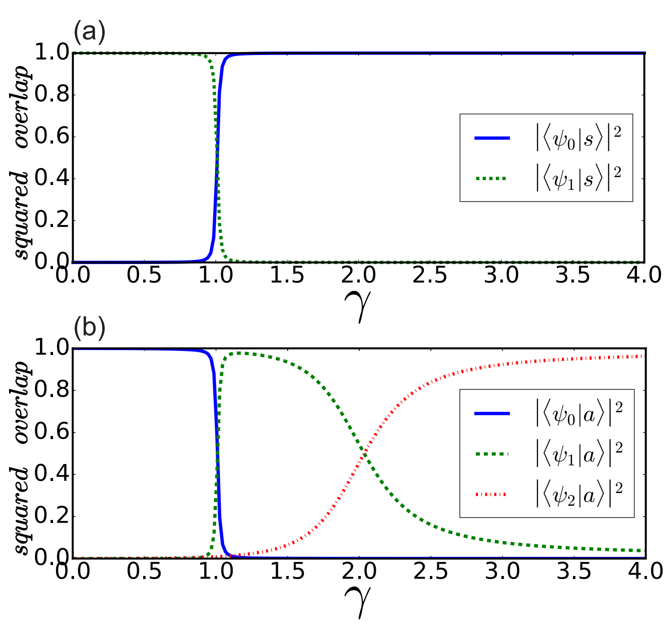

FIG. 6. The squared overlaps of basis states $|s\rangle$, $|a\rangle$ with the eigenstates $|\psi_{0,1}\rangle$ of H for a weighted balanced tree of height 2 when $\omega = M$.

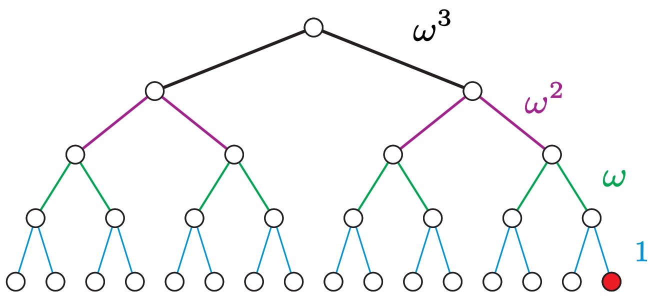

FIG. 7. Weighted balanced tree of height 4 and branching factor 2. The red vertex is the marked leaf vertex.

C. The case with a small M and a large r

Now, let us discuss the cases when the branching factor M is small while the height r is large. Interestingly, by properly adjusting the weights of edges between different levels [e.g., setting the weights to 1, ω, ω^2, ..., respectively, from bottom up (Fig. 7)], we can still achieve the optimal runtime and a high success probability for a small branching factor (Sec. IIID of Ref. [51]). Compared to a recent scheme [3] for this case, which gives a runtime proportional to N, our scheme provides a substantial speedup. The influence of the height r on the success probability P is shown in Fig. S12 (Sec. IIIE of Ref. [51]).

D. Quantum search on real trees

For the tree database similar to a real telephone directory, the graph could be very asymmetric and each branch could have a different branching factor (see Fig. 8). Surprisingly, for all the cases we have tried numerically, if the adjusted edge weight ω is large enough, we always find the marked leaf vertex with a runtime $\Theta(\sqrt{N})$ and a success probability close to 100% (see Sec. III F of Ref. [51] for details). Such a robust result makes the scheme of great practical significance to search on structured databases like real telephone directories.

V. FURTHER DISCUSSIONS

In our single-stage scheme, we need to modify the edge weights, i.e., increasing the edge weights close to the root.

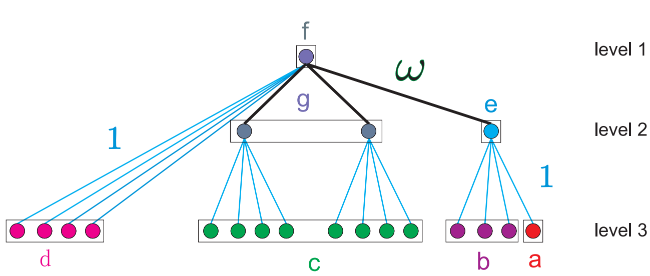

FIG. 8. A real tree could be a weighted tree with highly asymmetric structure, and the marked vertices could be any vertex on the bottom level. With a large weight ω between the first and the intermediate level, a fast search with optimal runtime $\Theta(\sqrt{N})$ and success probability close to 100% is always achieved in a large number of situations we have tried.

One might worry that this increase in edge weights could increase the energy consumption. However, actually our strategy to increase the edge weights does not increase the energy consumption, as we show that the state evolves mainly in a subspace with low energy as $\langle\psi(t)|H|\psi(t)\rangle = -\frac{1}{N}$ (details are given in Sec. IV A of Ref. [51]). The higher-energy levels act as both barriers and bridges for the probability to tunnel between the lower-energy levels. This magic tunneling is really fascinate!

Our results show that optimal quantum search can be achieved on intrinsically poorly connected graphs. A tree is intrinsically poorly connected since it becomes disconnected whichever edge is removed (the joined complete graphs [37] is not poorly connected in this sense). It has a low connectivity, irrespective of which measure one uses. According to the definition in Ref. [52], the average connectivity of the weighted balanced tree of height 2 when $\omega = M$ is roughly $4/N$. More discussions on different measures of connectivity can be found in Sec. IV B of Ref. [51].

In Ref. [33], an ingenious condition for quantum search via CTQW as well as a lower bound of the success probability was obtained, which however only guarantees a success probability of $\Theta(1/N^2)$ for the balanced trees with adjusted edge weights (see the discussion in Sec. IV C of Ref. [51]). To achieve a high success probability, one may need to repeat the search $\Theta(N^2)$ times, and the overall search is even slower than the classical scheme. However, via our scheme we actually achieve a probability close to 100%, which is independent of N, and our scheme can be accomplished in a single run with a runtime $\Theta(\sqrt{N})$. Trees with weighted edges have far richer structure of the Hilbert space in which one can design useful quantum algorithms.

We would like to briefly mention the possible implementation of our schemes. The two-dimensional CTQW has been demonstrated experimentally on a photonic chip [29]. The weight of edges of the corresponding graph, on which the photon performs quantum walk, is determined by the coupling strength between different waveguides. And one could actually control this coupling strength by engineering the waveguide spacing so as to implement the quantum walk on a particular graph. Since the way we modify the weight of the edges is highly symmetric, one might fabricate the waveguide arrays corresponding to the weighted tree by changing a certain group of the waveguide spacing while keeping the waveguide arrays regular enough to be experimentally feasible.

VI. CONCLUSIONS

We have discussed quantum search on structured databases, especially balanced trees with various heights and branching factors. Though balanced trees have low connectivity, our multistage quantum search scheme can achieve a success probability approaching 100%, which does not decrease even when the height or branching factor of the tree increases. By controlling the edge weights between different levels, we have a single-stage scheme and achieve an optimal runtime $\Theta(\sqrt{N})$ while keeping the high success probability. Both our multistage scheme for balanced trees and our single-stage scheme for trees with adjusted edge weights require only a single run to achieve the high success probability. We find that our controlled search scheme also works for real trees with unbalanced structures, and we expect similar results hold for other graphs with hierarchical structures. Finally, these schemes are also quite robust under small deviations of the jumping rates or small perturbation of the graph structure (Sec.V of Ref. [51]).

The usage of controllable edge weights may be unavoidable in order to fully release the magic power of quantum search on many structured databases, the same strategy may also be useful for quantum simulation [53] and other quantum information processing tasks.

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