Search algorithm on strongly regular graphs based on scattering quantum walks*

Xi-Ling Xue(薛希玲), Zhi-Hao Liu(刘志昊), and Han-Wu Chen(陈汉武)†

School of Computer Science and Engineering, Southeast University, Nanjing 210096, *China*

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Janmark, Meyer, and Wong showed that continuous-time quantum walk search on known families of strongly regular graphs (SRGs) with parameters (N,k,λ,μ) achieves full quantum speedup. The problem is reconsidered in terms of scattering quantum walk, a type of discrete-time quantum walks. Here, the search space is confined to a low-dimensional subspace corresponding to the collapsed graph of SRGs. To quantify the algorithm's performance, we leverage the fundamental pairing theorem, a general theory developed by Cottrell for quantum search of structural anomalies in star graphs. The search algorithm on the SRGs with k scales as N satisfies the theorem, and results can be immediately obtained, while search on the SRGs with k scales as $\sqrt{N}$ does not satisfy the theorem, and matrix perturbation theory is used to provide an analysis. Both these cases can be solved in $O(\sqrt{N})$ time steps with a success probability close to 1. The analytical conclusions are verified by simulation results on two SRGs. These examples show that the formalism on star graphs can be applied more generally.

Keywords: scattering quantum walk, quantum search, strongly regular graph

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1. Introduction

Quantum walk, the quantum mechanical counterpart of classical random walk, has been recently shown to constitute a universal model of quantum computation.[1–3] Defined by analogy to classical random walk, a quantum walk is a time-homogeneous quantum process on a graph. Both random and quantum walks can be defined either in continuous or discrete time. Continuous- and discrete-time quantum walks are introduced as counterparts of classical continuous- and discrete-time random walks, respectively. However, unlike their classical counterparts, the discrete-time walk cannot simply reduce to the continuous-time walk as a limiting case. Two important types of discrete-time quantum walks are coined quantum walk (CQW) and scattering quantum walk (SQW). CQWs are defined on vertices with an auxiliary coin space representing the directions of walking. In SQWs, the particle resides on the edges of the graph. These two types of walks are unitary equivalent.[4]

The search problem is a major concern in cloud computing[5–7] and quantum properties have been exploited to solve classical problems.[8,9] Quantum walks have been proven to be a useful framework in designing new quantum algorithms, the most notable of which are search algorithms.[10–17] Recent research have focused on the analysis of quantum search algorithms' performance. It is generally difficult to quantify the dynamics of search algorithms. Ambainis brought about a generalization of Grover's algorithm, the abstract search algorithm,[11,12] which characterizes the core of many existing search algorithms and ascertains their performance. Besides a general search for special vertices, recent studies have shown that quantum walks can also be used to find structural anomalies which affect a graph's symmetry.[18–20] A general formalism of a star graph S_N with another graph G attached to one of its external vertices was established to analyze the search of structural anomalies.[21,22] The overall graph is divided across the central vertex into two sides: G and the part which is connected to S_N constitute the right side, and the remainder of the S_N constitute the left side. Thus, the left side corresponds roughly to the initial state, which is intended to be rotated to the target state. It has been proven that these two sides must share the same eigenvalue when $N \to \infty$ to acquire a quadratic speedup, and quantum search helps to achieve this.

The topological structure plays an important role in quantum search algorithms on complete graphs, hypercubes and star graphs as well as in classical computer network.[23,24] In the quantum-walk-based algorithms, graph automorphism that commutes with the evolutionary operator $\boldsymbol{U}$ is used to identify the invariant subspace of the entire space. With a carefully chosen initial state, quantum walk on the original graph effectively evolves on a "collapsed graph" that corresponds to the subspace. It was believed that the ideal problem to be solved by a quantum walk would be a problem with global symmetry. The phenomenon of reducing effective dimension due to the symmetry of the graph was analysed in detail in Ref. [25]

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†Corresponding author. E-mail: hanwu_chen@163.com

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for CQW and in Ref. [13] for SQW. Most recent research disapproved this conjecture by demonstrating that search on the known strongly regular graphs (SRGs), which are believed to have no global symmetry for large N, acquires quadratic speedup.[15]

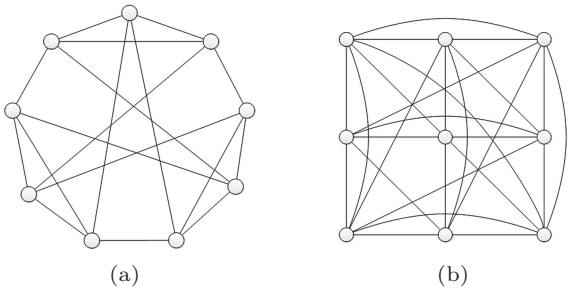
We consider a search algorithm on SRGs in terms of discrete-time quantum walks. To quantify the performance of the search algorithm, we first divide the SRGs into two types and then leverage the techniques and results in Refs. [21] and [22] to provide a detailed analysis. We present the simulation results on two SRGs to provide an intuitive illustration. Our results confirm the conjecture in Ref. [22] that the theory on star graphs can be applied more generally.

2. Preliminaries

The Hilbert space of scattering quantum walk on graph $G(V,E)$, with V being the set of vertices and E the set of edges, is defined as $H = l^2(\{|j,k\rangle : j,k \in V, jk \in E\})$, where jk is the edge connecting vertices j and k. Each edge corresponds to two states, i.e., one for each of the two possible directions. For each vertex $k (k \in V)$ in G, there are two subspaces A_k and Ω_k, which are spanned by the outgoing and incoming edges of k, respectively. Local unitary evolutions act as $U^k : \Omega_k \to A_k$, i.e., scattering on vertex k. The overall unitary operator $\boldsymbol{U}$ describing one step of SQW on graph G is the combined action of all the local unitary evolutions.

In a general search algorithm, there is a vertex which behaves differently from the others and the objective is to identify this target vertex. The local unitary operators act on vertex k as $\boldsymbol{U}^k|j,k\rangle = r_k|k,j\rangle + t_k \sum_{l\neq j} |k,l\rangle$, where r_k and t_k are reflection and transmission coefficients on vertex k, respectively. The target vertex reflects with a phase ϕ, which means that $r_k = \mathrm{e}^{\mathrm{i}\phi}$, $t_k = 0$. The phase shift operator acts as an oracle to mark the special vertex. An oracle is a black box that can recognize solutions to certain problems. In what follows ϕ is set to be π. For all the other vertices $r_k = 2/d_k - 1$, $t_k = 2/d_k$, where d_k is the degree of vertex k. This choice of local unitary operators is analogous to the choice of diffusive operator $\boldsymbol{G} = 2|\phi\rangle\langle\phi| - I$ in Grover's algorithm,[26] where $|\phi\rangle = (1/\sqrt{n}) \sum_{i=0}^{n-1} |i\rangle$ is the equal superposition of n states.

Definition 1 An SRG with parameters (N,k,λ,μ) is a graph G with N vertices, not complete or null, in which the number of common neighbours of x and y is k, λ, or μ depending on whether x and y are equal, adjacent or non-adjacent, respectively. If an SRG has parameters (N,k,λ,μ), then a necessary but insufficient constraint is that they satisfy $k(k-\lambda-1) = \mu(N-k-1)$.[15] Figure 1 shows two examples of SRGs.



(a) (b)

Fig. 1. (a) Paley graph with parameters (9,4,1,2), and (b) Latin square graph with parameters (9,6,3,6).

Definition 2 (N,k,λ,μ) is a Type-I parameter set if $2k = (N-1)(\mu-\lambda)$. Then since $N > 1+k$ and $\lambda \neq \mu$, we have $N = 4\mu+1$, $k = 2\mu$, $\lambda = \mu - 1$. The Paley graphs of order q are Type-I SRGs with parameters $(q,(q-1)/2,(q-5)/4,(q-1)/2)$, where q must be a prime power and be congruent to 1 mod 4.

In the Type-I SRGs, k scales as N, and there is another type where k scales less than N but no less than $\sqrt{N}$. The Latin square graphs with parameter set $(n^2, d(n-1), d^2-3d+n, d(d-1))$ are of this type. When $d = 2$, it is the $n \times n$ square lattice graph with parameters $(n^2, 2n-2, n-2, 2)$.

3. Search algorithm on SRGs

It is proved that "almost all" SRGs are asymmetric for large N. This means that their automorphism groups are trivial, and there is no automorphism taking a vertex to any other vertex. Thus, the method to collapse SRGs based on graph automorphism group, as given in Ref. [22], can no longer be applied. Nevertheless, we can construct an invariant subspace by the action of U on the graphs.

3.1. Collapsing SRGs

First let us group the three types of vertices together: the target vertex t, its k adjacent vertices, denoted as a, and the remaining $N-k-1$ vertices, denoted as b, which are not adjacent to the marked one. We then define the following edge states:

$$a \to t : |\psi_1\rangle = \frac{1}{\sqrt{k}} \sum_{i=1}^{k} |i,t\rangle, \tag{1}$$

$$t \to a : |\psi_2\rangle = \frac{1}{\sqrt{k}} \sum_{i=1}^{k} |t,i\rangle, \tag{2}$$

$$a \to a : |\psi_3\rangle = \frac{1}{\sqrt{k\lambda}} \sum_{i=1}^{k} \sum_{j=1}^{\lambda} |i,j\rangle, \tag{3}$$

$$\begin{aligned} a \to b : |\psi_4\rangle &= \frac{1}{\sqrt{k(k-\lambda-1)}} \sum_{i=1}^{k} \sum_{j=1}^{k-\lambda-1} |i,j\rangle \\ &= \frac{1}{\sqrt{(N-k-1)\mu}} \sum_{i=1}^{N-k-1} \sum_{j=1}^{\mu} |j,i\rangle, \end{aligned} \tag{4}$$

$$b \to a : |\psi_5\rangle = \frac{1}{\sqrt{(N-k-1)\mu}} \sum_{i=1}^{N-k-1} \sum_{j=1}^{\mu} |i,j\rangle$$

$$= \frac{1}{\sqrt{k(k-\lambda-1)}} \sum_{i=1}^{k} \sum_{j=1}^{k-\lambda-1} |j,i\rangle, \quad (5)$$

$$b \to b : |\psi_6\rangle = \frac{1}{\sqrt{(k-\mu)(N-k-1)}} \sum_{i=1}^{N-k-1} \sum_{j=1}^{k-\mu} |i,j\rangle, \quad (6)$$

These six states form a subspace of the Hilbert space, which we will see is invariant under the action of the unitary operator. The collapsed graph of SRGs is defined as follows: the vertex set is $\{t,a,b\}$, and the edge set is composed of edge sates $|\psi_1\rangle$ to $|\psi_6\rangle$, which correspond to directed edges *at*, *ta*, *aa*, *ab*, *ba*, *bb*, respectively, as shown in Fig. 2.

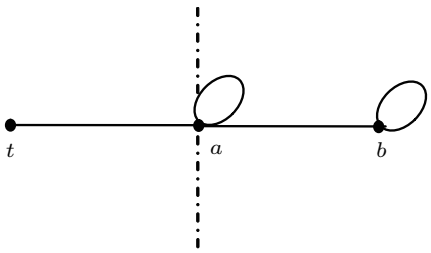


Fig. 2. Collapsed graph of SRGs.

The initial state is chosen to be an equal superposition of all the edge states in the original SRGs, and can be expressed as

$$\begin{aligned} &|\psi_{\text{init}}\rangle \\ &= \frac{1}{\sqrt{Nk}} \sum_{i=1}^{N} \sum_{j=1}^{k} |i,j\rangle \\ &= \frac{1}{\sqrt{N}}|\psi_1\rangle + \frac{1}{\sqrt{N}}|\psi_2\rangle + \sqrt{\frac{\lambda}{N}}|\psi_3\rangle + \sqrt{\frac{k-\lambda-1}{N}}|\psi_4\rangle \\ &\quad + \sqrt{\frac{k-\lambda-1}{N}}|\psi_5\rangle + \sqrt{\frac{(k-\mu)(N-k-1)}{Nk}}|\psi_6\rangle. \end{aligned} \quad (7)$$

Therefore, the initial state lies in the subspace.

As t is the target vertex, $\boldsymbol{U}|\psi_1\rangle = -|\psi_2\rangle$. A simple way to obtain the action of $\boldsymbol{U}$ on the other states is by considering the effect of the Grover diffusion operator. Local unitary operator on vertex v ($v \neq t$) mapping $\Omega_v \to A_v$ is $\boldsymbol{U}_v = 2|\varphi_v\rangle\langle\varphi_v| - \boldsymbol{I}_k$, where $|\varphi_v\rangle$ is the equal superposition of k edge states associated with v and $\boldsymbol{I}_k$ is the k-dimensional identity matrix. Each of the k adjacent vertices of vertex t has 1 edge connected to vertex t, λ connected to the other vertices in a, and the remaining $k-\lambda-1$ connected to the vertices in b. Thus, the 3D collapsed form of the k-dimensional $|\varphi_v\rangle$ associated with the collapsed vertex a is $|\varphi_a\rangle = (1/\sqrt{k}\ \sqrt{\lambda/k}\ \sqrt{(k-\lambda-1)/k})^{\mathrm{T}}$. The unitary operator on vertex a mapping $\Omega_a \to A_a$ takes the form

$$\begin{aligned} &\boldsymbol{U}_a = 2|\varphi_a\rangle\langle\varphi_a| - \boldsymbol{I}_3 \\ &= \begin{pmatrix} \frac{2}{k}-1 & \frac{2\sqrt{\lambda}}{k} & \frac{2\sqrt{k-\lambda-1}}{k} \\ \frac{2\sqrt{\lambda}}{k} & \frac{2\lambda}{k}-1 & \frac{2\sqrt{\lambda(k-\lambda-1)}}{k} \\ \frac{2\sqrt{k-\lambda-1}}{k} & \frac{2\sqrt{\lambda(k-\lambda-1)}}{k} & 1-\frac{2(\lambda+1)}{k} \end{pmatrix}. \end{aligned}$$

Similarly, we can obtain the unitary operator on the collapsed vertex b as

$$\boldsymbol{U}_b = \begin{pmatrix} \frac{2\mu}{k}-1 & \frac{2\sqrt{\mu(k-\mu)}}{k} \\ \frac{2\sqrt{\mu(k-\mu)}}{k} & 1-\frac{2\mu}{k} \end{pmatrix}.$$

Thus, in the basis $\{|\psi_1\rangle,|\psi_2\rangle,|\psi_3\rangle,|\psi_4\rangle,|\psi_5\rangle,|\psi_6\rangle\}$, the unitary operator $\boldsymbol{U}$ on the subspace can be expressed as

$$\boldsymbol{U} = \begin{pmatrix} 0 & \frac{2}{k}-1 & \frac{2\sqrt{\lambda}}{k} & 0 & \frac{2\sqrt{k-\lambda-1}}{k} & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{2\sqrt{\lambda}}{k} & \frac{2\lambda}{k}-1 & 0 & \frac{2\sqrt{\lambda(k-\lambda-1)}}{k} & 0 \\ 0 & \frac{2\sqrt{k-\lambda-1}}{k} & \frac{2\sqrt{\lambda(k-\lambda-1)}}{k} & 0 & 1-\frac{2(\lambda+1)}{k} & 0 \\ 0 & 0 & 0 & \frac{2\mu}{k}-1 & 0 & \frac{2\sqrt{\mu(k-\mu)}}{k} \\ 0 & 0 & 0 & \frac{2\sqrt{\mu(k-\mu)}}{k} & 0 & 1-\frac{2\mu}{k} \end{pmatrix}. \quad (8)$$

It is easy to verify that $\boldsymbol{U}^{\dagger}\boldsymbol{U} = \boldsymbol{I}$. To quantify the performance, we divide the problem into two cases: when k scales as N and when k scales less than N, but not less than $\sqrt{N}$ from the definition of SRGs. We will see in the following subsections that the $k = \Theta(N)$ case can be solved using Cottrell's formalism, while the $k = o(N)$ case cannot, and we resort to the matrix perturbation theory.

3.2. The $k = \Theta(N)$ case

Let us give a brief review of techniques and results in Refs. [21] and [22]. Star graph S_N with an unspecified graph G attached to one of the external vertices is divided into left

and right segments, with the central vertex acting as a hub. For a general value of N denote operator $\boldsymbol{U}$ as $\boldsymbol{U}(\varepsilon)$, the perturbation variable $\varepsilon = 1/N$ in this case. When $N \to \infty$, the leading-order matrix of $\boldsymbol{U}(\varepsilon)$ is $\boldsymbol{U}(0)$, a block diagonal matrix with two blocks $\boldsymbol{U}_{0,\mathrm{L}}$ and $\boldsymbol{U}_{0,\mathrm{R}}$ corresponding to the two sides. Considering the λ_0-eigenspace of $\boldsymbol{U}(0)$, the left (right) λ_0 eigenvector refers to eigenvector native to $\boldsymbol{U}_{0,\mathrm{L}}(U_{0,\mathrm{R}})$. The λ_0 eigenvector is called an active eigenvector if it will be affected when moving from the $\varepsilon = 0$ case to the $\varepsilon \neq 0$ case. There is a unique active eigenvector on each side of the hub vertex corresponding to eigenvalue λ_0, denoted as $|\iota_0\rangle$ and $|\tau_0\rangle$.

Fundamental pairing theorem[22] The λ_0-eigenspace is in contact with both the left and right sides of the hub vertex if and only if there exist paired vectors $|v_\pm\rangle$ with eigenvalues of the form $\lambda_\pm = \lambda_0 \mathrm{e}^{\pm \mathrm{i}c\sqrt{\varepsilon}} + O(\sqrt{\varepsilon})$, where $c = \lim\limits_{\varepsilon\to 0}(1/\sqrt{\varepsilon})|\langle\iota_0|\boldsymbol{U}|\tau_0\rangle|$. With correctly chosen complex phases, the paired eigenvectors take the form $|v_\pm\rangle = (1/\sqrt{2})(|\iota_0\rangle \pm |\tau_0\rangle) + O(\sqrt{\varepsilon})$.

It was also shown that the optimal number of time steps for a search is $m = \lfloor \pi/2c\sqrt{\varepsilon} \rfloor$, and the probability of the state being either in G or on the edge between G and the hub is $1 - O(\sqrt{\varepsilon})$.

The above formalism can be used to analyze structural anomalies in complete graphs.[20] Here is another application. The collapsed graph of SRGs in Fig. 2 is divided into two parts: the left part consists of vertex t, vertex a, and the collapsed edge between t and a; the right part consists of vertex a, the loops on a, vertex b, the loops on b, and the collapsed edge between a and b. Thus, the right part corresponds roughly to the initial state, which is intended to be rotated to the target states, $|\psi_1\rangle$ and $|\psi_2\rangle$.

We consider Type-I SRGs. With $N = 4\mu + 1$, $k = 2\mu$, $\lambda = \mu - 1$, the expression of $\boldsymbol{U}$ in Eq. (8) becomes

$$\boldsymbol{U} = \begin{pmatrix} 0 & \frac{1}{\mu} - 1 & \frac{\sqrt{\mu-1}}{\mu} & 0 & \frac{1}{\sqrt{\mu}} & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{\mu-1}}{\mu} & -\frac{1}{\mu} & 0 & \sqrt{\frac{\mu-1}{\mu}} & 0 \\ 0 & \frac{1}{\sqrt{\mu}} & \sqrt{\frac{\mu-1}{\mu}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}. \tag{9}$$

Let $\boldsymbol{U}(\varepsilon) = \boldsymbol{U}(0) + \sqrt{\varepsilon}\boldsymbol{A}_1 + \cdots$, $\varepsilon = 1/\mu$, the leading- and first-order terms of $\boldsymbol{U}(\varepsilon)$ in Eq. (9) are, for large μ,

$$\boldsymbol{U}(0) = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix},$$

$$\boldsymbol{A}_1 = \begin{pmatrix} 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The characteristic polynomial of $\boldsymbol{U}(0)$ is $|\lambda \boldsymbol{I} - \boldsymbol{U}(0)| = (\lambda-1)^2(\lambda+1)^2(\lambda^2+1)$. It turns out that the only interesting eigenvalue is $\lambda_0 = 1$, with right active eigenvector $|\tau_0\rangle = (|\psi_3\rangle + |\psi_4\rangle + |\psi_5\rangle + |\psi_6\rangle)/2$ and left active eigenvector $|\iota_0\rangle = (1/\sqrt{2})(|\psi_1\rangle - |\psi_2\rangle)$. Thus, the paired eigenvectors of $\boldsymbol{U}$ are $|v_\pm\rangle = (1/\sqrt{2})(\mp i|\iota_0\rangle + |\tau_0\rangle) + O(\sqrt{\varepsilon}) = (1/\sqrt{2})(\mp \mathrm{i}/\sqrt{2} \;\; \pm \mathrm{i}/\sqrt{2} \;\; 1/2 \;\; 1/2 \;\; 1/2 \;\; 1/2)^{\mathrm{T}} + O(\sqrt{\varepsilon})$. $c = |\langle\iota_0|\boldsymbol{A}_1|\tau_0\rangle| = 1/\sqrt{2}$; therefore, we have $\lambda_\pm = \lambda_0 \mathrm{e}^{\pm \mathrm{i}c\sqrt{\varepsilon}} + O(\varepsilon) = \mathrm{e}^{\pm \mathrm{i}\sqrt{\varepsilon/2}} + O(\varepsilon)$. The initial state can be expressed as a superposition of two eigenvectors $|\psi_{\mathrm{init}}\rangle = |\tau\rangle + O(\sqrt{\varepsilon}) = (1/\sqrt{2})(|v_+\rangle + |v_-\rangle) + O(\sqrt{\varepsilon})$. The optimal number of time steps for the search is $m = \lfloor \pi\sqrt{N}/2\sqrt{2} \rfloor$, and the probability of the state being on the edge connected to the target vertex is $1 - O(N^{-1/2})$.

Another double root of the characteristic polynomial of $\boldsymbol{U}_0$ is -1, with eigenvector $|v_0\rangle = (1/2\sqrt{2})(\sqrt{2} \;\; \sqrt{2} \;\; 1 \;\; -1 \;\; -1 \;\; 1)^{\mathrm{T}}$. However, in this case, the initial state has little overlap with the eigenspace spanned by the corresponding eigenvector, i.e., $\langle v_0|\psi_{\mathrm{init}}\rangle \approx 0$. In addition, the root is constant, which means it will not be affected by perturbation.

3.3. The $k = o(N)$ case

As for $k = o(N)$, we take the Latin square graph $\mathrm{srg}(n^2, 2n-2, n-2, 2)$ for example. The unitary operator $\boldsymbol{U}$ reads

$$\boldsymbol{U} = \begin{pmatrix} 0 & \frac{1}{n-1} - 1 & \frac{\sqrt{n-2}}{n-1} & 0 & \frac{1}{\sqrt{n-1}} & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{n-2}}{n-1} & -\frac{1}{n-1} & 0 & \sqrt{\frac{n-2}{n-1}} & 0 \\ 0 & \frac{1}{\sqrt{n-1}} & \sqrt{\frac{n-2}{n-1}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2}{n-1} - 1 & 0 & \frac{2\sqrt{n-2}}{n-1} \\ 0 & 0 & 0 & \frac{2\sqrt{n-2}}{n-1} & 0 & 1 - \frac{2}{n-1} \end{pmatrix}. \tag{10}$$

For large n, the leading-order terms of $\boldsymbol{U}$ in Eq. (10) are

$$\boldsymbol{U}(0) = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

The characteristic polynomial of $\boldsymbol{U}(0)$ is $(\lambda-1)^2(\lambda+1)^2(\lambda^2-\lambda+1)$. The double root -1 of $\boldsymbol{U}_0$ is a constant root and the associated eigenvector $|v_0\rangle = (1/2 \quad 1/2 \quad 1/\sqrt{6} \quad -1/\sqrt{6} \quad -1/\sqrt{6} \quad 0)^{\mathrm{T}}$ has little overlap with the initial state. The only interesting eigenvalue is $\lambda_0 = 1$ and its corresponding eigenvectors are $|\tau_0\rangle = |\psi_6\rangle$ and $|\iota_0\rangle = (1/\sqrt{2})(|\psi_1\rangle - |\psi_2\rangle)$ for the right and left sides, respectively. Since $|\tau_0\rangle$ is not in contact with the hub vertex a, we cannot use the fundamental pairing theorem to obtain the eigenspectrum of the evolutionary operator. It makes sense because if the theorem holds, we would acquire quadratic speedup over $n = \sqrt{N}$.

The state of the walk after m steps is derived by employing the decomposition formula $|\psi_m\rangle = \sum_{\lambda} \lambda^m \langle v_\lambda|\psi_{\mathrm{init}}\rangle |v_\lambda\rangle$, where $|v_\lambda\rangle$ are the orthogonal eigenvectors corresponding to the eigenvalue λ of the unitary operator $\boldsymbol{U}$. The typical approach to diagonalize $\boldsymbol{U}$ involves a perturbative approach to finding the eigenvalues and eigenstates, which is shown as follows. Although the pattern of calculation is basic, it involves tedious calculations. It can also be applied to the analysis of Type-I SRGs, which is included in the Appendix A.

For simplicity, we replace $n-1$ with n, for large n. The characteristic polynomial of Eq. (10) is

$$\lambda^6 - \frac{n-3}{n}\lambda^5 - \frac{n^2-2}{n^2}\lambda^4 + \frac{2(n-1)(n-2)}{n^2}\lambda^3 - \frac{n^2-2}{n^2}\lambda^2 - \frac{n-3}{n}\lambda + 1 = 0,$$

which can be rewritten as

$$(\lambda+1)^2\left(\lambda^4 - \frac{3(n-1)}{n}\lambda^3 + \frac{2(n-1)(2n-1)}{n^2}\lambda^2 - \frac{3(n-1)}{n}\lambda + 1\right) = 0. \tag{11}$$

Set $\lambda = \Delta + 1$, and substitute it back into the fourth-order equation for λ in Eq. (11). Keeping only the lowest-order term, we obtain $n^2\Delta^2 + 4\Delta + 2 = 0$, with roots $\Delta = \pm\sqrt{2}\varepsilon i$, where $\varepsilon = 1/n$. Let $\theta = \sqrt{2}\varepsilon$, the eigenvalues can be expressed as $\lambda_\pm = \mathrm{e}^{\pm \mathrm{i}\theta} + O(\varepsilon)$, with corresponding eigenvectors $|v_\pm\rangle = (1/\sqrt{3})(1 \quad -1 \quad 0 \quad 0 \quad 0 \quad \pm 1) + O\left(\sqrt{\varepsilon}\right)$. The initial state can also be expressed as a superposition of two eigenvectors

$$\begin{aligned}|\psi_{\mathrm{init}}\rangle &= \frac{1}{n}(|\psi_1\rangle + |\psi_2\rangle) + \frac{\sqrt{n-2}}{n}|\psi_3\rangle \\ &\quad + \frac{\sqrt{n-1}}{n}(|\psi_4\rangle + |\psi_5\rangle) \\ &\quad + \frac{\sqrt{(n-1)(n-2)}}{n}|\psi_6\rangle \\ &= |\tau\rangle + O(\sqrt{\varepsilon}) \\ &= \frac{1}{\sqrt{2}}(|v_+\rangle - |v_-\rangle) + O(\sqrt{\varepsilon}).\end{aligned}$$

Applying $\boldsymbol{U}$ repeatedly for m times yields

$$\begin{aligned}&\boldsymbol{U}^m|\psi_{\mathrm{init}}\rangle \\ &= \frac{1}{\sqrt{2}}(\lambda_+^m|v_+\rangle - \lambda_-^m|v_-\rangle) \\ &= \frac{1}{\sqrt{6}}[(\mathrm{e}^{\mathrm{i}m\theta} \quad -\mathrm{e}^{\mathrm{i}m\theta} \quad 0 \quad 0 \quad 0 \quad \mathrm{e}^{\mathrm{i}m\theta})^{\mathrm{T}} \\ &\quad - (\mathrm{e}^{-\mathrm{i}m\theta} \quad -\mathrm{e}^{-\mathrm{i}m\theta} \quad 0 \quad 0 \quad 0 \quad -\mathrm{e}^{-\mathrm{i}m\theta})^{\mathrm{T}}] + O(\sqrt{\varepsilon}) \\ &= \sqrt{\frac{2}{3}}\mathrm{i}(\sin(m\theta) \quad -\sin(m\theta) \quad 0 \quad 0 \quad 0 \quad \cos(m\theta))^{\mathrm{T}} + O(\sqrt{\varepsilon}).\end{aligned}$$

Starting from $|\psi_{\mathrm{init}}\rangle$, after $m = \lfloor n\pi/2\sqrt{2}\rfloor = \lfloor \pi\sqrt{N}/2\sqrt{2}\rfloor$ time steps, the particle is located on one of the edges connecting to target vertex with success probability $1 - O(N^{-1/4})$. The time complexity of these two examples is the same; however, the success probability of Latin square graphs is lower than that of Type-I SRGs

3.4. Simulation results

To intuitively illustrate the evolutionary process of the search algorithm, this subsection presents the numerical simulation results. Numerical simulation also allows us to compare the actual scaling with the bounds proved previously. First, consider the Paley graph with parameters (121, 60, 29, 30). We substitute the parameter set into Eqs. (7) and (8) to obtain the initial state and the evolutionary operator, respectively, of the search algorithm on SRG (121, 60, 29, 30) as

$$|\psi_{\mathrm{init}}\rangle = (\,0.0909 \;\; 0.0909 \;\; 0.4895 \;\; 0.4979 \;\; 0.4979 \;\; 0.4979\,)^{\mathrm{T}},$$

$$\boldsymbol{U} = \begin{pmatrix} 0 & -0.9667 & 0.1795 & 0 & 0.1826 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.1795 & -0.0333 & 0 & 0.9832 & 0 \\ 0 & 0.1826 & 0.9832 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

Figure 3 plots the results of simulating our algorithm for an increasing number of time steps.

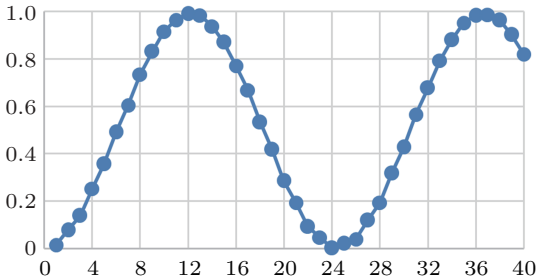


Fig. 3. (color online) Probability of marked state over 40 time steps on SRG (121,60,29,30).

To compare with the case in Section 3.3, we repeat the simulation process on an SRG with the same number of vertices as the Latin square graph with parameters (121, 20, 9, 2). Similarly, the initial state and the evolutionary operator can be obtained by substituting the parameter set (121, 20, 9, 2) into Eqs. (7) and (8), respectively. So we have

$|\psi_{\text{init}}\rangle = (0.0909 \quad 0.0909 \quad 0.2727 \quad 0.2875 \quad 0.2875 \quad 0.8624)^{\text{T}}$, and

$$\boldsymbol{U} = \begin{pmatrix} 0 & -0.9 & 0.3 & 0 & 0.3162 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.3 & -0.09 & 0 & 0.9487 & 0 \\ 0 & 0.3162 & 0.9487 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.8 & 0 & 0.6 \\ 0 & 0 & 0 & 0.6 & 0 & 0.8 \end{pmatrix}.$$

Figure 4 shows the simulation results of the relationship between the number of iterations and the success probability.

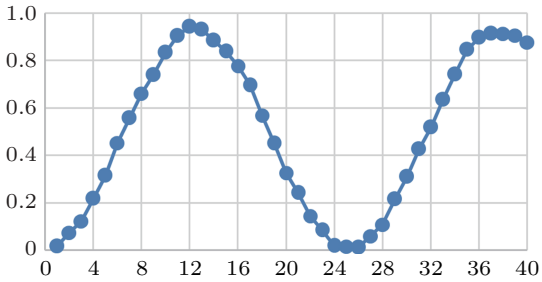


Fig. 4. (color online) Probability of marked state over 40 time steps on SRG (121, 20, 9, 2).

As the evolutionary operator is unitary, the success probability changes quasi-periodically with the time evolution, which is confirmed by Figs. 3 and 4. In both the figures, the probability of the walkers being located on an edge connected to the target vertex are first amplified by the oracle operation until reaching the peak at $t = 12$ time steps, which is consistent with the analytical time complexity $\lfloor \pi\sqrt{N}/2\sqrt{2} \rfloor$. The maximum success probability is affected by the graph structure, with the former a little higher than the latter. This is consistent with the analytical results presented above, i.e., $1 - O(N^{-1/2})$ for the Paley Graphs and $1 - O\left(N^{-1/4}\right)$ for the Latin square graphs.

4. Discussion and conclusion

Set $\boldsymbol{U}_1$ in the abstract search algorithm as $\boldsymbol{U}_1 = \boldsymbol{I} - 2|\psi_1\rangle\langle\psi_1|$, $\boldsymbol{U}_2 = \boldsymbol{U}\boldsymbol{U}_1$. Thus, $\boldsymbol{U}_1|\psi_1\rangle = -|\psi_1\rangle$ and it leaves any state orthogonal to $|\psi_1\rangle$ unchanged. $\boldsymbol{U}_2|\psi_{\text{init}}\rangle = |\psi_{\text{init}}\rangle$, and all the other eigenvectors of $\boldsymbol{U}_2$, denoted as $|\varphi_i\rangle$, satisfy $\langle\psi_{\text{init}}|\phi_i\rangle = 0$ and $U_2|\phi_i\rangle = \mathrm{e}^{\mathrm{i}\theta}|\varphi_i\rangle$, for $\theta \in [\varepsilon, 2\pi - \varepsilon]$, where ε is determined by the parameter set (N, k, λ, μ). Thus, the search algorithm on SRGs with parameters (N, k, λ, μ) is an instance of abstract search algorithm. However, the success probability depends on phase gap ε and thus it depends on parameter set (N, k, λ, μ), which is consistent with results presented in Section 3. We intend further study how these parameters influence the success probability.

It is proved that "almost all" SRGs are asymmetric for large N. Nevertheless, we can construct an invariant subspace by the action of $\boldsymbol{U}$ on the graphs. It means that the existence of invariant evolutionary subspace may not necessarily depend on the global symmetry. Vertices in SRGs that are not structurally equivalent may evolve synchronously, which is consistent with the results in Refs. [27] and [28]. By confining the search space within a six-dimensional invariant subspace, we show that scattering quantum walk search algorithm on all SRGs with parameters (N, k, λ, μ) can be solved with time complexity $O(\sqrt{N})$. Our results indicate that the techniques and results in Refs. [21] and [22] can be applied more generally than star graphs, and which other situations it can be applied to is a question of great interest.

Appendix A

The characteristic polynomial of $\boldsymbol{U}$ in Eq. (9) is

$$\lambda^6 + \frac{1}{\mu}\lambda^5 - \frac{\mu-1}{\mu}\lambda^4 - \frac{\mu-1}{\mu}\lambda^2 + \frac{1}{\mu}\lambda + 1 = 0,$$

i.e.,

$$(\lambda+1)^2\left(\lambda^4 - \frac{2\mu-1}{\mu}\lambda^3 + \frac{2\mu-1}{\mu}\lambda^2 - \frac{2\mu-1}{\mu}\lambda + 1\right) = 0. \tag{A1}$$

When $\mu \gg 1$, the zeroth-order polynomial is $(\lambda+1)^2(\lambda-1)^2(\lambda^2+1) = 0$. Set $\lambda = \Delta + 1$, and substitute it back into the fourth-order equation for λ in Eq. (A1). Keeping only the lowest-order term, we find $2\mu\Delta^2 + 2\Delta + 1 = 0$, whose roots are $\Delta = \pm\mathrm{i}\sqrt{\varepsilon}/\sqrt{2}$, where $\varepsilon = 1/\mu$. Thus the eigenvalues are $\lambda_\pm = 1 \pm \mathrm{i}/\sqrt{2\mu} + O(\varepsilon)$ with associated eigenvectors $|v_\pm\rangle = (1/\sqrt{2})(\mp\mathrm{i}/\sqrt{2} \quad \pm\mathrm{i}/\sqrt{2} \quad 1/2 \quad 1/2 \quad 1/2 \quad 1/2)^{\text{T}} + O(\sqrt{\varepsilon})$. The initial state is approximately equal to a superposition of two eigenvectors,

$$\begin{aligned} |\psi_{\text{init}}\rangle &= \frac{1}{\sqrt{4\mu+1}}(|\psi_1\rangle + |\psi_2\rangle) + \sqrt{\frac{\mu-1}{4\mu+1}}|\psi_3\rangle \\ &\quad + \sqrt{\frac{\mu}{4\mu+1}}(|\psi_4\rangle + |\psi_5\rangle + |\psi_6\rangle) \\ &= |\tau\rangle + O(\sqrt{\varepsilon}) \\ &= \frac{1}{\sqrt{2}}(|v_+\rangle + |v_-\rangle) + O(\sqrt{\varepsilon}). \end{aligned}$$

Applying $\boldsymbol{U}$ repeatedly for m times yields

$$\begin{aligned} \boldsymbol{U}^m|\psi_{\text{init}}\rangle &= \frac{1}{\sqrt{2}}\left(\lambda_+^m|v_+\rangle + \lambda_-^m|v_-\rangle\right) + O(\sqrt{\varepsilon}) \\ &= \frac{1}{2\sqrt{2}}\begin{pmatrix} -\sqrt{2}\mathrm{i}\left(\mathrm{e}^{\mathrm{i}m\theta} - \mathrm{e}^{-\mathrm{i}m\theta}\right) \\ \sqrt{2}\mathrm{i}\left(\mathrm{e}^{\mathrm{i}m\theta} - \mathrm{e}^{-\mathrm{i}m\theta}\right) \\ \mathrm{e}^{\mathrm{i}m\theta} + \mathrm{e}^{-\mathrm{i}m\theta} \\ \mathrm{e}^{\mathrm{i}m\theta} + \mathrm{e}^{-\mathrm{i}m\theta} \\ \mathrm{e}^{\mathrm{i}m\theta} + \mathrm{e}^{-\mathrm{i}m\theta} \\ \mathrm{e}^{\mathrm{i}m\theta} + \mathrm{e}^{-\mathrm{i}m\theta} \end{pmatrix} + O(\sqrt{\varepsilon}) \end{aligned}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} -\sqrt{2}\mathrm{i}\sin m\theta \\ \sqrt{2}\mathrm{i}\sin m\theta \\ \cos m\theta \\ \cos m\theta \\ \cos m\theta \end{pmatrix} + O(\sqrt{\varepsilon}).$$

From the expression, we see that the probability amplitudes for edge states connected to target vertex are approximately equal to one when $m\theta = \pi/2$. If we measure the position of the particle after $m = O(\sqrt{N})$ steps, it will, with probability $1 - O(\sqrt{\varepsilon})$, be located on an edge connected to the target vertex.

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