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Quantitative approach to Grover's quantum walk on graphs

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Abstract

In this paper, we study Grover's search algorithm focusing on continuous-time quantum walk on graphs. We propose an alternative optimization approach to Grover's algorithm on graphs that can be summarized as follows: Instead of finding specific graph topologies convenient for the related quantum walk, we fix the graph topology and vary the underlying graph Laplacians. As a result, we search for the most appropriate analytical structure on graphs endowed with fixed topologies yielding better search outcomes. We discuss strategies to investigate the optimality of Grover's algorithm and provide an example with an easy tunable graph Laplacian to investigate our ideas.

Keywords Grover's quantum walk · Weighted directed graphs · Probabilistic graph Laplacian

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1 Introduction

Quantum search algorithms on graphs have a subtle relationship to the connectivity of the graph. Completely connected graphs and topologies with bridges between completely connected components provided configuration space for efficient quantum search [32] realizations. Search based on joined complete graphs can be realized with atomic systems interacting with an environment bringing such scheme closer to reality [49]. In a recent work, Pan et al., have shown that classical electric circuits perform on par with graph-based quantum search algorithm [43]. The electrical circuit-based approach can be generalized to perform search on multiple sites simultaneously[28]. In this work, we consider a different family of weighted graphs with self-similar structure for the configuration space quantum search algorithms. Advances in development of fractal configurations in physical systems suggest ways to implement quantum walk propagation on fractal graphs. For example, Fusco et al. [24] realized fractal geometries in photonic metamaterials, and on such lattices, it may be possible to implement a quantum walk protocol developed by Kitagawa et al. [31] to perform Grover's search.

The theory of quantum algorithms has been an active area of study over the last three decades, see [16, 38, 39, 44] and references therein. In several applications, quantum algorithms have been shown to outperform their classical counterparts, hence leading to a speedup in performance [26, 46]. In this paper, we revisit Grover's search algorithm [1, 9, 10, 17, 20, 26, 45, 48], focusing on the continuous-time quantum walk approach developed by [15, 23]. The Childs–Goldstone approach is very versatile and can be realized on quantum systems of different geometrical or topological arrangements. This feature appeared in [18, 34, 35] where it was established that a certain class of fractal-type graphs demonstrates favorable topological properties to implement perfect quantum state transfer. The feature is also present in [2], where Grover's search algorithm was analyzed on databases with different topological arrangements. In this latter case, the (analytical and numerical) investigations of quantum walk on several graphs, such as the dual Sierpinski gaskets, T-fractals and hierarchical structures like Cayley trees, illustrate the dependency of Grover's algorithm on the topological structure of these graphs.

In this paper, we propose an alternative optimization approach to Grover's algorithm on graphs. In particular, instead of finding specific graph topologies convenient for the related quantum walk, we fix the graph topology and vary the underlying graph Laplacians. As a result, we search for the most appropriate analytical structure on graphs endowed with fixed topologies yielding better outcomes in Grover's search algorithm. To describe our approach's main ideas, we first introduce some basic terminology and notation. We perform a Grover's search on a database modeled by a finite (possibly directed) graph $G = (V, E)$. Let $\{p(x, y)\}_{(x,y)\in E}$ be a sequence of weights assigned to the edges, where we regard the edge (x, y) as pointing from the vertex x to y and $p(x, y)$ as a transition probability of a quantum walker from x to y.

We impose the following conditions

$$\begin{cases} (x, y) \in E \;\Leftrightarrow\; 0 < p(x, y) \leq 1 \\ (x, y) \notin E \;\Leftrightarrow\; p(x, y) = 0 \\ \sum_{y:(x,y)\in E} p(x, y) = 1, \;\forall\, x \in V \end{cases} \tag{1}$$

and associate with such a sequence a *probabilistic graph Laplacian* on G, defined by

$$\Delta_G f(x) = f(x) \;-\; \sum_{y:(x,y)\in E} p(x, y) f(y). \tag{2}$$

We assume there exists a Hilbert space $\big(\mathcal{H}, \langle ., . \rangle\big)$ such that Δ_G is self-adjoint (Hermitian),

$$\langle \Delta_G \psi, \phi \rangle = \langle \psi, \Delta_G \phi \rangle, \quad \phi, \psi \in \mathcal{H} = \big\{ f : V \to \mathbb{C} \big\}.$$

We refer to [37] for more details and for examples of such Hilbert spaces on certain graphs. We associate each item in the database with a vertex $x \in V$ or equivalently the corresponding normalized Dirac function

$$e_x := \delta_x / \sqrt{\langle \delta_x, \delta_x \rangle}, \qquad \delta_x(y) := \begin{cases} 1, & x = y \\ 0, & x \neq y \end{cases}$$

and denote the target vertex in Grover's search algorithm by $w \in V$. Note that $\mu : V \to (0, \infty)$, $\mu(x) := \langle \delta_x, \delta_x \rangle$ defines a measure on the set of vertices V. The *volume* of the graph G is then given by

$$vol(G) := \sum_{x\in V} \mu(x), \quad \mu(x) = \langle \delta_x, \delta_x \rangle. \tag{3}$$

To perform the search, one needs a driving Hamiltonian H of the quantum system. In this work, we use (see [2, 15])

$$\begin{cases} H_\gamma := \gamma \Delta_G - V_w, \\ V_w f := \langle e_w, f \rangle e_w, \quad f : V(G) \to \mathbb{C}, \end{cases} \tag{4}$$

where γ is a tunable parameter in $(0, \infty)$. The potential operator V_w is also called the *oracle Hamiltonian*. As the initial state of the search, we choose the ground state of Δ_G

$$s := \frac{1}{\sqrt{vol(G)}} \sum_{x\in V(G)} \delta_x \tag{5}$$

and the goal is to evolve s continuously to the target state e_w. The success probability of finding the target vertex w at the time t is then given by

$$\pi_w^\gamma(t) := \left|\langle e_w, \exp(-i H_\gamma t)s\rangle\right|^2. \tag{6}$$

Our main contribution is summarized as follows. Rather than investigating a family of Hamiltonians $\{H_\gamma\}_{\gamma\in(0,\infty)}$ on graphs of different topologies, we fix the (topology on) graph G and vary the transition probabilities (1) of a quantum walker on G. By doing so, we are effectively varying Δ_G in (2). As such, we are led to the following question: "Can we construct examples for which this approach improves Grover's search outcomes?". In Sect. 3, we provide an example with an easy tunable parameter to answering this question.

The rest of the paper is organized as follows: In Sect. 2, we will discuss strategies to investigate the optimality of Grover's search algorithm. We recall that the algorithm is implemented using a family of Hamiltonians $\{H_\gamma\}_{\gamma\in(0,\infty)}$ for which one is led to determine in a systematic manner the value γ_{opt} for which $H_{\gamma_{opt}}$ leads to optimal search outcomes, i.e., $\pi_w^{\gamma_{opt}}(t)$ is maximal in the shortest time possible (see (33) for the definition of γ_{opt}). In [15], Childs and Goldstone elaborated on the interplay between the success probability (6) and the overlap probabilities

$$|\langle s, \psi_0\rangle|^2,\ |\langle e_w, \psi_0\rangle|^2,\ |\langle s, \psi_1\rangle|^2,\ |\langle e_w, \psi_1\rangle|^2, \tag{7}$$

where ψ_0 (resp. ψ_1) refer to the ground (resp. first excited) state of H_γ. As such, we focus on a better understanding of these overlap probabilities resulting in our first main contribution Theorem 2.3. This result provides conditions (15) under which we can approximate and relate the ψ_0-eigenvalue E_0 (resp. ψ_1-eigenvalue E_1) with the square root of the graph's volume, i.e.,

$$E_0 \approx -\frac{\sqrt{\langle \delta_w, \delta_w\rangle}}{\sqrt{vol(G)}}, \quad E_1 \approx \frac{\sqrt{\langle \delta_w, \delta_w\rangle}}{\sqrt{vol(G)}}. \tag{8}$$

We point out that for the complete graph on N vertices the eigenvalues are given by

$$E_0 = -\frac{1}{\sqrt{N}}, \quad E_1 = \frac{1}{\sqrt{N}}, \tag{9}$$

and the sufficient conditions Theorem 2.3 are satisfied. Furthermore, in this case we have $\langle \delta_w, \delta_w\rangle = 1$ for all $w \in V$ and $vol(G) = N$ is nothing else but the number of vertices.

In practice, it might be difficult to verify (15) for general graphs. Therefore, we introduced the parameter γ_E in (14) for which the corresponding success probability $\pi_w^{\gamma_E}(t)$ takes the simple form (25). In fact, for a complete graph on N vertices we have $\gamma_E = \gamma_{opt}$ holds for all N, and hence, the corresponding optimal success probability is easily computed using (25) and given by

$$\pi_w^{\gamma_{opt}}(t) = \left(\frac{N-1}{N}\right)\sin^2\left(\frac{t}{\sqrt{N}}\right) + \frac{1}{N}. \tag{10}$$

These observations have led us to the second part of this work: Does the equality $\gamma_{opt} = \gamma_E$ hold for other graphs? Or more specifically, is it possible to construct a graph such that the following properties hold:

$$\begin{cases} \text{A graph with variable volume} vol(G). \\ \text{The optimal success probability is well approximated by(25).} \\ E_1 \text{ is well approximated by} \frac{\sqrt{\langle \delta_w, \delta_w \rangle}}{\sqrt{vol(G)}}. \end{cases} \tag{11}$$

In Sect. 3, we introduce a hypercubic lattice as a Cartesian product of directed path graphs. To keep the discussion simple, we assume that the path graph has four vertices and that the transition probabilities of a quantum walker between these vertices are given via a parameter p, see Figs. 1 and 2. This parameter p can be interpreted as quantifying the database homogeneity/non-homogeneity and will play the role of the tuning parameter of the graph volume $vol(G)$. Despite the simplicity of this model, we obtain interesting results when investigating the properties (11).

Our work is part of a long term study of mathematical physics on fractals and self-similar graphs [3–8, 21, 27, 40–42], in which novel features of quantum processes on fractals can be associated with the unusual spectral and geometric properties of fractals compared to regular graphs and smooth manifolds.

2 Continuous-time quantum walk on finite graphs

We start this section with some preliminary results that will be needed later for the proof of Proposition 2.2 and Theorem 2.3. Let E_a and ψ_a denote the eigenvalues and eigenvectors of H_γ, respectively. We assume that $\{\psi_a\}_{E_a \in \sigma(H_\gamma)}$ is an orthonormal basis and in this notation, E_0 and ψ_0 refer to the ground state, E_1 and ψ_1 refer to the first excited state, and so on. For ease of discussion, we will assume in this work that E_0 and E_1 are non-degenerate. For $\gamma > 0$ and $z \in \rho(\gamma\Delta_G)$, the resolvent set of $\gamma\Delta_G$, we consider the following Green function

$$G_\gamma(z, w, w) := \langle e_w, (\gamma\Delta_G - z)^{-1} e_w \rangle. \tag{12}$$

Let $\{\phi_\lambda \mid \lambda \in \sigma(\Delta_G)\}$ be an orthonormal basis of eigenvectors of Δ_G, and write

$$e_w = \sum_{\lambda \in \sigma(\Delta_G)} a_{w,\lambda}\phi_\lambda, \qquad a_{w,\lambda} = \langle \phi_\lambda, e_w \rangle. \tag{13}$$

where the sum takes the eigenvalue multiplicities into account. The following result whose proof we omit is elementary.

Lemma 2.1 *The following statements hold.*

1. *If* $E_a \notin \sigma(\gamma \Delta_G)$, *then* $\langle e_w, \psi_a\rangle \neq 0$.
2. *If* $E_a \notin \sigma(\gamma \Delta_G)$, *then* $G_\gamma(E_a, w, w) = 1$.
3. *If* $E_a \notin \sigma(\gamma \Delta_G)$, *then* $\langle e_w, (\gamma\Delta_G - E_a)^{-1}\psi_a\rangle = \frac{1}{\langle \psi_a, e_w\rangle}$.
4. *If* $z \in \rho(\gamma\Delta_G)$, *then*

$$\begin{cases} G_\gamma(z, w, w) = \sum_{\lambda\in\sigma(\Delta_G)} \frac{|a_{w,\lambda}|^2}{\gamma\lambda - z} \\ G'_\gamma(z, w, w) = \frac{d}{dz}G_\gamma(z, w, w) = \sum_{\lambda\in\sigma(\Delta_G)} \frac{|a_{w,\lambda}|^2}{(\gamma\lambda - z)^2} = \langle e_w, (\gamma\Delta_G - z)^{-2}e_w\rangle. \end{cases}$$

Next, for general finite graphs we derive formulas for the overlap probabilities.

Proposition 2.2 *(Overlap probabilities) Suppose that* $E_a \notin \sigma(\gamma\Delta_G)$. *Then we have*

1. $|\langle e_w, \psi_a\rangle|^2 = \frac{1}{G'_\gamma(E_a, w, w)}$.
2. $|\langle s, \psi_a\rangle|^2 = \frac{\langle \delta_w, \delta_w\rangle}{vol(G)E_a^2 G'_\gamma(E_a, w, w)}$.

Proof The proof uses Lemma 2.1.

1. Given that $\psi_a = \langle e_w, \psi_a\rangle(\gamma\Delta_G - E_a)^{-1}e_w$, we have

$$\begin{aligned} 1 = \langle \psi_a, \psi_a\rangle &= \overline{\langle e_w, \psi_a\rangle}\langle e_w, \psi_a\rangle\langle e_w, (\gamma\Delta_G - E_a)^{-2}e_w\rangle \\ &= \langle e_w, (\gamma\Delta_G - E_a)^{-2}e_w\rangle|\langle e_w, \psi_a\rangle|^2 \end{aligned}$$

The statement follows by Lemma 2.1(4).

2. Recalling that $\Delta_G s = 0$, we see that

$$-E_a\langle s, \psi_a\rangle = \langle s, (\gamma\Delta_G - E_a)\psi_a\rangle = \langle s, V_w\psi_a\rangle = \langle s, e_w\rangle\langle e_w, \psi_a\rangle.$$

Hence, $|\langle s, \psi_a\rangle|^2 = \frac{|\langle s, e_w\rangle|^2\, |\langle e_w, \psi_a\rangle|^2}{E_a^2}$ and the result follows by $|\langle s, e_w\rangle|^2 = \frac{\langle \delta_w, \delta_w\rangle}{vol(G)}$ and part (1).

□

To study the question of which parameter γ the Hamiltonian H_γ leads to optimal search outcomes, we will consider the following parameters with the assumption that each of the sets below is non-empty

$$\begin{cases} \gamma_s := \inf_{\gamma\in(0,\infty)} \left\{\gamma \;\middle|\; \text{such that } |\langle s, \psi_0\rangle|^2 = |\langle s, \psi_1\rangle|^2\right\} \\ \gamma_w := \inf_{\gamma\in(0,\infty)} \left\{\gamma \;\middle|\; \text{such that } |\langle e_w, \psi_0\rangle|^2 = |\langle e_w, \psi_1\rangle|^2\right\}. \\ \gamma_E := \inf_{\gamma\in(0,\infty)} \left\{\gamma \;\middle|\; \text{such that } E_0 = -E_1\right\}. \end{cases} \tag{14}$$

The following theorem establishes a relationship between the overlap probabilities and the eigenvalues E_0, E_1 and provides sufficient conditions to approximate these eigenvalues by the square root of the graph's volume.

Theorem 2.3 *Assume that there exist $\gamma \in (0, \infty)$ and $\epsilon > 0$ such that*

$$\Big| |\langle s, \psi_0\rangle|^2 - |\langle e_w, \psi_0\rangle|^2 \Big| \le \epsilon. \tag{15}$$

Then

$$\left| E_0^2 - \frac{\langle \delta_w, \delta_w\rangle}{vol(G)} \right| \le \epsilon.$$

Similarly, if the inequality (15) holds for ψ_1, then

$$\left| E_1^2 - \frac{\langle \delta_w, \delta_w\rangle}{vol(G)} \right| \le \Big(1 + \frac{\langle \delta_w, \delta_w\rangle}{vol(G)} \frac{||\langle s, \psi_1\rangle|^2 - |\langle s, \psi_0\rangle|^2|}{|\langle s, \psi_1\rangle|^2 |\langle s, \psi_0\rangle|^2}\Big)\epsilon.$$

Proof By Proposition 2.2(2), we have

$$\left| E_a^2 - \frac{\langle \delta_w, \delta_w\rangle}{vol(G)} \right| = \frac{\langle \delta_w, \delta_w\rangle}{vol(G)} \left| \frac{1 - G'_\gamma(E_a, w, w)|\langle s, \psi_a\rangle|^2}{G'_\gamma(E_a, w, w)|\langle s, \psi_a\rangle|^2} \right| \tag{16}$$

$$= \frac{\langle \delta_w, \delta_w\rangle}{vol(G)} \left| \frac{|\langle e_w, \psi_a\rangle|^2 - |\langle s, \psi_a\rangle|^2}{|\langle s, \psi_a\rangle|^2} \right| \tag{17}$$

$$= E_a^2 G'_\gamma(E_a, w, w) \Big| |\langle e_w, \psi_a\rangle|^2 - |\langle s, \psi_a\rangle|^2 \Big|, \tag{18}$$

where in the second equality, we used $1 = G'_\gamma(E_a, w, w)|\langle e_w, \psi_a\rangle|^2$ (see Proposition 2.2(1)), and in the last equality, we used Proposition 2.2(2). The result follows from the following computations. First, we note that Lemma 2.1(4), $E_0 < 0$ and $\sigma(\Delta_G) \subset [0, 2]$ show

$$E_0^2 G'_\gamma(E_0, w, w) = E_0^2 \sum_{\lambda \in \sigma(\Delta_G)} \frac{|a_{w,\lambda}|^2}{(\gamma\lambda + |E_0|)^2} \tag{19}$$

$$\le \sum_{\lambda \in \sigma(\Delta_G)} |\langle \phi_\lambda, e_w\rangle|^2 = ||e_w||^2 = 1. \tag{20}$$

Moreover, Proposition 2.2 (2) shows

$$\left| E_1^2 G'_\gamma(E_1, w, w) - E_0^2 G'_\gamma(E_0, w, w) \right| = \frac{\langle \delta_w, \delta_w\rangle}{vol(G)} \frac{\Big| |\langle s, \psi_1\rangle|^2 - |\langle s, \psi_0\rangle|^2 \Big|}{|\langle s, \psi_1\rangle|^2 |\langle s, \psi_0\rangle|^2}. \tag{21}$$

□

Complete graphs are examples for which the hypotheses of Theorem 2.3 are satisfied. In fact, if we consider the probabilistic graph Laplacian of a complete graph of N

vertices

$$\Delta_G = \begin{pmatrix} 1 & -\frac{1}{N-1} & \cdots & \cdots & -\frac{1}{N-1} \\ -\frac{1}{N-1} & 1 & -\frac{1}{N-1} & \cdots & -\frac{1}{N-1} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & -\frac{1}{N-1} & 1 & -\frac{1}{N-1} \\ -\frac{1}{N-1} & \cdots & \cdots & -\frac{1}{N-1} & 1 \end{pmatrix}, \tag{22}$$

and set $\gamma = \frac{N-1}{N}$, then a direct computation of the overlap probabilities gives

$$\begin{cases} |\langle s, \psi_0 \rangle|^2 = |\langle e_w, \psi_0 \rangle|^2 = \frac{\sqrt{N}+1}{2\sqrt{N}} \\ |\langle s, \psi_1 \rangle|^2 = |\langle e_w, \psi_1 \rangle|^2 = \frac{\sqrt{N}-1}{2\sqrt{N}}. \end{cases} \tag{23}$$

It follows that (15) holds for any $\epsilon > 0$, the eigenvalues are given by (9), and that, by definition, we have $\gamma_E = \frac{N-1}{N}$. We remark that the Hamiltonian in [2, 15] is defined using the graph Laplacian $D - A$, where D (resp. A) is the degree (resp. adjacency) matrix of the graph. By the regularity of complete graphs, the probabilistic graph Laplacian (22) coincides with the graph Laplacian up to a multiple constant, i.e., $(N-1)\Delta = (D - A)$. Using either operators has no impact on the analysis since

$$\gamma \Delta - V_w = \tilde{\gamma}(D - A) - V_w$$

where $\gamma = (N-1)\tilde{\gamma}$. In particular, $\gamma = \gamma_E = \frac{N-1}{N}$ if and only if $\tilde{\gamma} = \frac{1}{N}$, in which case, as proved in [15], a quantum search on complete graphs recovers the optimal quadratic speedup. Therefore, for complete graphs, Theorem 2.3 implies that $E_0 = -E_1$. The following result gives the consequences of assuming that $E_0 = -E_1$ for a given graph with a fixed topology.

Proposition 2.4 *Suppose that there exists $\gamma \in (0, \infty)$ such that $E_0 = -E_1$, then*

$$\frac{|\langle e_w, \psi_1 \rangle|^2}{|\langle s, \psi_1 \rangle|^2} = \frac{|\langle e_w, \psi_0 \rangle|^2}{|\langle s, \psi_0 \rangle|^2}. \tag{24}$$

Consequently, we have $\overline{\langle \psi_1, s \rangle} \langle e_w, \psi_0 \rangle = -e^{i2\theta} \overline{\langle \psi_0, s \rangle} \langle e_w, \psi_1 \rangle$ for some phase $\theta \in [0, \pi)$. Moreover, the success probability reduces to

$$\pi_w^{\gamma}(t) = 4|\langle s, \psi_0 \rangle|^2 \, |\langle e_w, \psi_1 \rangle|^2 \sin^2(E_1 t + \theta) + C + R(t) \tag{25}$$

where C and $R(t)$ are given by

$$\begin{cases} C := |\langle e_w, \psi_0 \rangle|^2 |\langle s, \psi_0 \rangle|^2 + |\langle e_w, \psi_1 \rangle|^2 |\langle s, \psi_1 \rangle|^2 - 2|\langle s, \psi_0 \rangle|^2 \, |\langle e_w, \psi_1 \rangle|^2 \\ R(t) := 2Re\big(A(t)\overline{r(t)}\,\big) + |r(t)|^2 \end{cases} \tag{26}$$

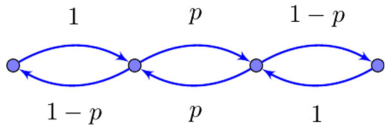

Fig. 1 Graph G and the corresponding probabilistic graph Laplacian Δ_G. When $p = 1/2$, Δ_G becomes the standard probabilistic graph Laplacian

with

$$\begin{cases} A(t) := \langle e_w, \psi_0\rangle\langle\psi_0, s\rangle \exp(-iE_0 t) + \langle e_w, \psi_1\rangle\langle\psi_1, s\rangle \exp(-iE_1 t) \\ r(t) := \sum_{a\geq 2}\langle e_w, \psi_a\rangle\langle\psi_a, s\rangle \exp(-iE_a t). \end{cases} \tag{27}$$

Proof The first result follows by Proposition 2.2 (1) & (2). To prove the second result, we use $\langle e_w, \exp(-itH_\gamma)s\rangle = A(t) + r(t)$ and compute

$$\begin{aligned} \pi_w^\gamma(t) = &|\langle e_w, \psi_0\rangle|^2|\langle s, \psi_0\rangle|^2 + |\langle e_w, \psi_1\rangle|^2|\langle s, \psi_1\rangle|^2 \\ &+ \langle e_w, \psi_0\rangle\langle\psi_0, s\rangle\overline{\langle e_w, \psi_1\rangle}\,\overline{\langle\psi_1, s\rangle}\exp(i(E_1 - E_0)t) \\ &+ \overline{\langle e_w, \psi_0\rangle}\,\overline{\langle\psi_0, s\rangle}\langle e_w, \psi_1\rangle\langle\psi_1, s\rangle\exp(-i(E_1 - E_0)t) \\ &+ A(t)\overline{r(t)} + \overline{A(t)}r(t) + r(t)\overline{r(t)}. \end{aligned}$$

Using the first result, we add the second and third terms together

$$\begin{aligned} -|\langle s, \psi_0\rangle|^2\,|\langle e_w, \psi_1\rangle|^2\exp(i2(E_1t+\theta)) - |\langle s, \psi_0\rangle|^2\,|\langle e_w, \psi_1\rangle|^2\exp(-i2(E_1t+\theta)) \\ = -2|\langle s, \psi_0\rangle|^2\,|\langle e_w, \psi_1\rangle|^2\cos(2(E_1t+\theta)) \\ = 4|\langle s, \psi_0\rangle|^2\,|\langle e_w, \psi_1\rangle|^2\sin^2(E_1t+\theta) - 2|\langle s, \psi_0\rangle|^2\,|\langle e_w, \psi_1\rangle|^2. \end{aligned}$$

□

3 Hypercubic lattices

In this section, we introduce a one-parameter family of Laplacians on the hypercubic lattice and investigate Grover's search algorithm numerically when using these Laplacians. Given a finite directed path graph $G = (V, E)$ with the vertices $V := \{0, 1, 2, 3\}$ and the edges $E := \{(x, y) \in V \times V \mid |x - y| = 1\}$. We consider a quantum walk on G, where the transition probabilities $\{p(x, y)\}_{(x,y)\in V\times V}$ and the corresponding probabilistic graph Laplacian Δ_G are given for some $p \in (0, 1)$ in Fig. 1. Note that Δ_G generates a quantum walk on G with reflecting boundaries. This class of Laplacians was first investigated in [47] and arises naturally when studying the unit interval endowed with a particular fractal measure. For more on this Laplacian and some related work, we refer to [11, 13, 14, 19, 36].

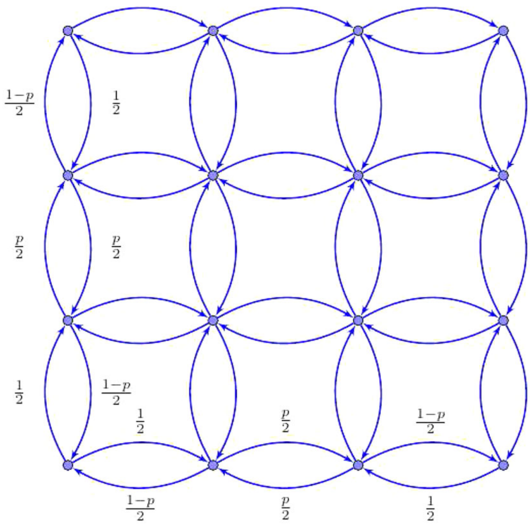

Fig. 2 Graph $G_2 = G' \times G''$, where $G' = G'' = G$ and G is the graph in Fig. 1. The transition probabilities are given by Δ_{G_2}

We equip the vertices set V with a measure, $\mu : V \to [0, \infty)$ and assume that it satisfies the Kolmogorov's cycle condition [22, 25, 29, 30], i.e.,

$$\mu(0) = 1, \quad \mu(x) = \mu(x-1)\frac{p(x-1,x)}{p(x,x-1)}, \quad x \in V. \tag{28}$$

One can easily verify that Δ_G is self-adjoint (Hermitian) with respect to the inner product

$$\langle f, g\rangle_G = \sum_{x\in V} \overline{f(x)}g(x)\mu(x), \tag{29}$$

where $f, g \in \mathcal{H}_G := span\{\ \delta_x \mid x \in V\}$. A *d-dimensional hypercubic lattice* is constructed as the d-fold Cartesian product of finite directed path graphs $G_d = G' \times G'' \times ..$, where $G' = G'' = \ldots = G$. For simplicity, we restrict our illustration to products of two graphs as the extension to higher-dimensional products is straightforward. We follow [12] and denote by a prime anything having to do with the first graph and by a double prime anything having to do with the second graph. We recall that a Cartesian product of two graphs $G' = (V', E')$ and $G'' = (V'', E'')$ is a graph $G_2 = G' \times G''$ with the set of vertices $V(G_2) = \{(x', x'') \mid x' \in V', x'' \in V''\}$, where two vertices $\bar{x} = (x', x'')$ and $\bar{y} = (y', y'')$ are adjacent, i.e., $(\bar{x}, \bar{y}) \in E(G_2)$ if and only if $(x', y') \in E'$ and $x'' = y''$ or $(x'', y'') \in E''$ and $x' = y'$. We define a Laplacian on G_2 as a (normalized) Kronecker sum of $\Delta_{G'}$ and $\Delta_{G''}$, i.e.,

$$\Delta_{G_2} := \frac{1}{2}\big(\Delta_{G'} \otimes I + I \otimes \Delta_{G''}\big), \tag{30}$$

where I is an identity matrix. An example of the quantum walk generated by Δ_{G_2} is illustrated in Fig. 2. We associate each vertex $\bar{x} = (x', x'') \in V(G_2)$ with $\delta_{\bar{x}} := \delta_{x'} \otimes \delta_{x''}$, the tensor product $\delta_{x'}$ and $\delta_{x''}$. It follows that Δ_{G_2} is self-adjoint on the Hilbert space $\mathcal{H}_{G_2} = span\{\, \delta_{\bar{x}} |\ \bar{x} = (x', x'') \in V(G_2)\,\}$ equipped with the inner product

$$\langle f, g\rangle = \sum_{\bar{x}\in V(G_2)} \overline{f(\bar{x})} g(\bar{x})\mu_2(\bar{x}), \quad \begin{cases} \langle \delta_{\bar{x}}, \delta_{\bar{y}}\rangle := \langle \delta_{x'}, \delta_{y'}\rangle_{G'} \langle \delta_{x''}, \delta_{y''}\rangle_{G''} \\ \mu_2(\bar{x}) := \langle \delta_{\bar{x}}, \delta_{\bar{x}}\rangle \end{cases} \tag{31}$$

3.1 Homogeneous versus non-homogeneous structures

When $p = \frac{1}{2}$, then Δ_{G_d} recovers the standard probabilistic graph Laplacian as a generator of a symmetric quantum walk on G_d. In this case, it easy to compute that the symmetrizing measure (31) is the degree of the vertex, i.e.,

$$\mu_d(\bar{x}) = \langle \delta_{\bar{x}}, \delta_{\bar{x}}\rangle = \mu(x_1)\ldots\mu(x_d) = 2^d,$$

where $\bar{x} = (x_1, \ldots, x_d) \in V(G_d)$ is a non-boundary vertex. In particular, the measure is constant on the interior vertices, and as such, we say that G_d *homogeneous*. On the other hand, when $p \neq \frac{1}{2}$, then Δ_{G_d} generates an asymmetric quantum walk on G_d. Consequently, the measure is vertex-dependent and varies on the interior vertices. In this case, we say G_d is *non-homogeneous*. For an interpretation from a physics viewpoint and the relation to fractal media, the reader is referred to the introduction of [14].

3.2 Numerical results

In this section, we present some numerical results on the Grover's search algorithm on the graph G_5 and provide the python codes in [33]. Note that the number of vertices is $|V(G_5)| = 1024$. The target vertex $w \in V(G_5)$ is assumed to be one of the corners of G_5. Our focus is to analyze the search algorithm based on the homogeneity versus non-homogeneity of the database, i.e., $p = 1/2$ versus $p \neq 1/2$. To this end, we plot the overlap probabilities and the eigenvalues E_0, E_1 as functions of γ, after which we determine and discuss their intersections at the points γ_s, γ_w and γ_E. Before proceeding, it is worth mentioning that for the complete graph of N vertices, where $N \geq 2$, we have $\gamma_s \leq \gamma_E \leq \gamma_w$. When $N = 2$, we have $\gamma_s = 0$ and $\gamma_w = \infty$, while for large N, we see that

$$\gamma_s \approx \gamma_E \approx \gamma_w \approx 1. \tag{32}$$

In the case of G_5, the plots of the overlap probabilities are depicted for several p in Fig. 3. The case $p = 0.91$ (top left panel in Fig. 3) is particularly interesting and is qualitatively similar to the results for the complete graphs; see [15, Figure 1] for a

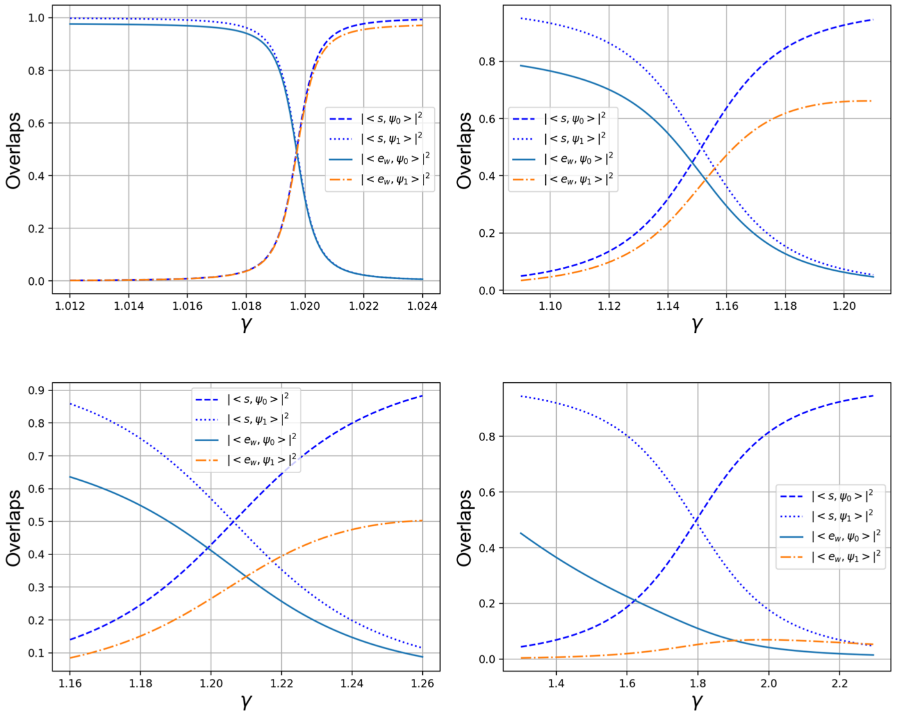

Fig. 3 Overlap probabilities as a function of γ for G_5: (top left) $p = 0.91$, (top right) $p = 0.5$, (bottom left) $p = 0.4$, (bottom right) $p = 0.1$

Table 1 Numerical computation of γ_s, γ_w, γ_E and γ_{opt} for G_5 and different values of p

p	γ_s	γ_w	γ_E	γ_{opt}
0.91	1.0197	1.0197	1.0197	1.0195
0.5	1.1515	1.1528	1.1521	1.1520
0.4	1.2063	1.2099	1.2081	1.2061
0.1	1.7935	1.9035	1.8438	1.785

comparison. We determine γ_s, γ_w and γ_E in Table 1, and observe that in all cases

$$\gamma_s \leq \gamma_E \leq \gamma_w,$$

where for larger p, γ_E is increasingly squeezed between γ_s and γ_w.

We also compute the success probability $\pi_w^\gamma(t)$ as a function of the time t and γ, see Fig. 4. Then we determine for which values (t, γ) the success probability $\pi_w^\gamma(t)$ is optimal, i.e.,

$$(t_{opt}, \gamma_{opt}) := \inf_{\gamma} \inf_{t} \left\{(t, \gamma) \in [0, vol(G)] \times (0, \infty) : \pi_w^\gamma(t) \text{ attains abs. max.}\right\}. \tag{33}$$

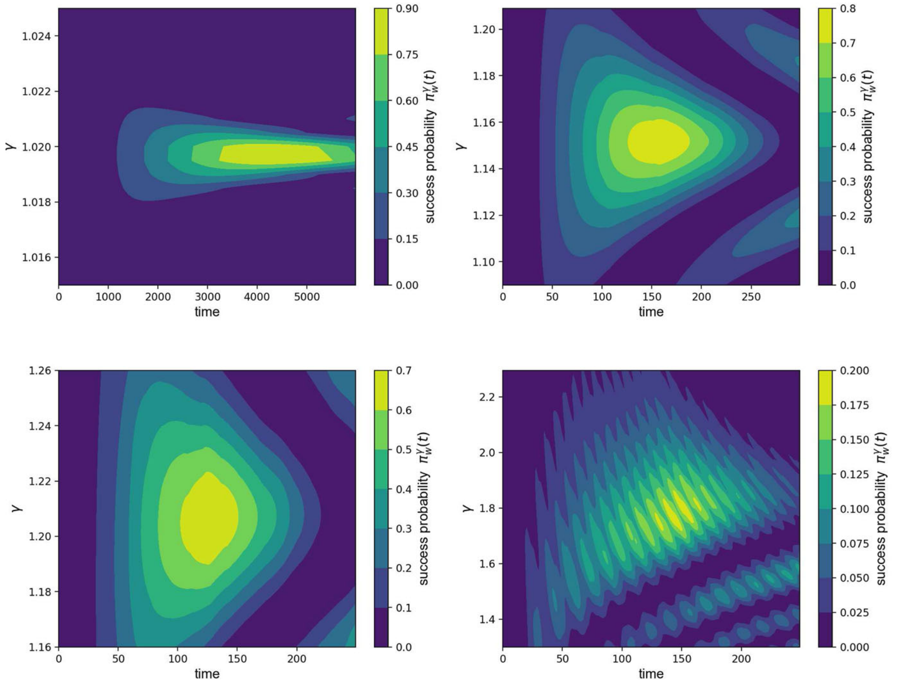

Fig. 4 Contour plot of the success probability $\pi_w^\gamma(t)$ as a function of the time t and γ for G_5: (top left) $p = 0.91$, (top right) $p = 0.5$, (bottom left) $p = 0.4$, (bottom right) $p = 0.1$

We observe that for $p = 0.91$, we have $\gamma_{opt} \approx \gamma_E \approx \gamma_s \approx \gamma_w$, see Table 1. (Note that for the complete graph of N vertices, we have $\gamma_{opt} = \gamma_E$ for any $N \geq 2$.) Subsequently, we determine E_0 and E_1 as the eigenvalues of the ground and first excited state of $H_{\gamma_{opt}}$. For comparison, we also compute $\sqrt{\frac{\langle \delta_w, \delta_w \rangle}{vol(G_5)}}$ using

$$vol(G_5) = \left(2 + \frac{2}{1-p}\right)^5.$$

Note that $\langle \delta_w, \delta_w \rangle = 1$ for w located at one of the corners of G_5. Again, the results for E_0 and E_1 are in better agreement with $\sqrt{\frac{\langle \delta_w, \delta_w \rangle}{vol(G_5)}}$ the larger we choose p. We plot the success probability $\pi_w^\gamma(t)$ as a function of t, where we set $\gamma = \gamma_{opt}$, see Fig. 5. Concerning the observation that $\gamma_{opt} \approx \gamma_E$ for $p = 0.91$, we note that the graph in the top left panel in Fig. 5 is in very good agreement with the analytical formula (25), i.e.,

$$\pi_w^{\gamma_{opt}}(t) \approx 0.89 \sin^2(E_1 t) \tag{34}$$

where the value of E_1 is given in Table 2. In contrast to the complete graphs where $\gamma_{opt} = \gamma_E$ holds for any number of vertices, we observe in G_5 that the deviation of γ_E from γ_{opt} increases for smaller values of p. In this case, formula (25) is less suitable

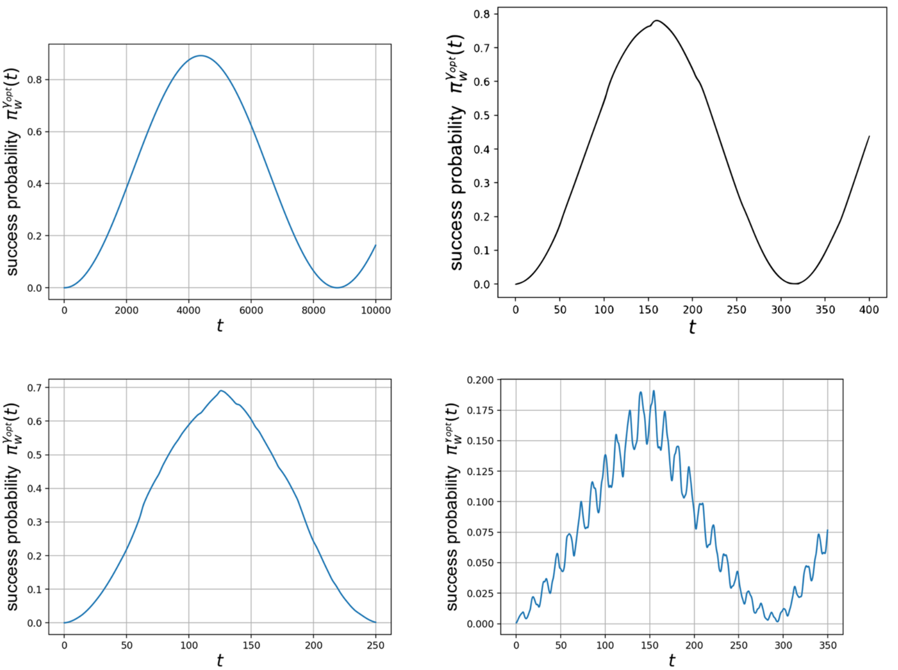

Fig. 5 Plot of the success probability $\pi_w^{\gamma}(t)$ as a function of time t for G_5. We set $\gamma = \gamma_{opt}$ in all panels: (top left) $p = 0.91$, (top right) $p = 0.5$, (bottom left) $p = 0.4$, (bottom right) $p = 0.1$

Table 2 Numerical computation of E_0, E_1, t_{opt} and $\frac{\pi}{2}\sqrt{\frac{vol(G_5)}{\langle\delta_w,\delta_w\rangle}}$ for G_5 and different values of p

p	E_0	E_1	$\sqrt{\frac{\langle\delta_w,\delta_w\rangle}{vol(G_5)}}$	t_{opt}	$\frac{\pi}{2}\sqrt{\frac{vol(G_5)}{\langle\delta_w,\delta_w\rangle}}$
0.91	−0.0004	0.0002	0.0003	4380	4535.8
0.5	−0.010	0.0099	0.0113	159.4	138.52
0.4	−0.0130	0.01189	0.0152	125.8	103.18
0.1	−0.0135	0.0085	0.0273	154.6	57.54

for analyzing of $\pi_w^{\gamma_{opt}}(t)$. Indeed, Fig. 5 (bottom right panel) illustrates how $\pi_w^{\gamma_{opt}}(t)$ for $p = 0.1$ exhibits a more irregular and oscillatory behavior.

Finally, we observe that t_{opt} decreases with (large) p and is comparable to $\frac{\pi}{2}\sqrt{\frac{vol(G_5)}{\langle\delta_w,\delta_w\rangle}}$, see Table 2. For example, $\pi_w^{\gamma_{opt}}(t)$ for $p = 0.91$ attains its maximum at $t_{opt} \approx 4380$, which is not practical for searching a database of 1024 elements. On the other hand, Fig. 6 seems to suggest that choosing smaller p might improve the optimal time of Grover's search algorithm. For example, when $p = 0.4$, we observe a slight improvement from the homogeneous case $p = 0.5$, see the corresponding t_{opt} values in Table 2. However, it seems that this improvement in Grover's optimal time is lost when p get smaller, e.g., see the case $p = 0.1$ in Table 2.

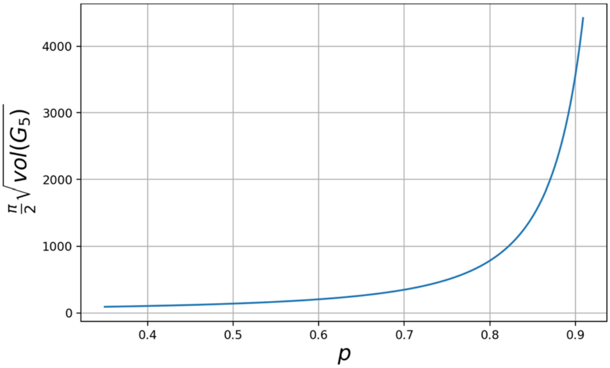

Fig. 6 Square root of the graph volume as a function of p for G_5

4 Conclusions

In this paper, we discussed strategies for the application of Childs–Goldstone approach [15] to Grover's quantum walk on graphs. A database is modeled by a finite (possibly directed) graph G, and the search algorithm is implemented using the family of Hamiltonians $\{H_\gamma\}_{\gamma\in(0,\infty)}$ in (4). Theorem 2.3 provides conditions (15) on the overlaps probabilities that are sufficient to approximate and relate the eigenvalues E_0, E_1 with the square root of the graph's volume. Complete graphs are examples for which the conditions (15) hold for $\gamma = \frac{N-1}{N}$ and any $\epsilon > 0$, but this is not the case for the hypercubic lattices, see, for instance, the top right panel in Fig. 3 (the homogeneous case $p = 0.5$). On the other hand, we were able to tune the overlap probabilities on hypercubic lattices by inducing non-homogeneity measured by the parameter p. Indeed, the top left panel in Fig. 3 evidences for $p = 0.91$ the existence of γ for which we have

$$|\langle s, \psi_0\rangle|^2 \approx |\langle e_w, \psi_0\rangle|^2 \approx |\langle s, \psi_1\rangle|^2 \approx |\langle e_w, \psi_1\rangle|^2.$$

To deal with graphs for which it might be unfeasible to check (15), we introduced γ_E (14) resulting in a simplified formula for the corresponding success probability $\pi_w^{\gamma_E}(t)$ (25). In particular, to understand $\pi_w^{\gamma_E}(t)$, we need to analyze the following quantities: E_1, $R(t)$ and the overlap probabilities

$$|\langle s, \psi_0\rangle|^2,\ |\langle e_w, \psi_0\rangle|^2,\ |\langle s, \psi_1\rangle|^2,\ |\langle e_w, \psi_1\rangle|^2.$$

This can be done rigorously for the complete graph of N vertices, where $\gamma_E = \frac{N-1}{N}$ and $\pi_w^{\gamma_E}(t)$ is given by (10). Furthermore, complete graphs are particularly interesting as $\gamma_E = \gamma_{opt}$, i.e., H_{γ_E} leads to optimal search outcomes. We then ask whether equality $\gamma_{opt} = \gamma_E$ hold for other graphs, or whether we can construct a graph for which the properties (11) hold.

For this, we propose an approach for optimizing Grover's algorithm on hypercubic lattice graphs. In particular, in Sect. 3, we fix the graph topology (as hypercubic lattices) and instead vary the analysis structure on these graphs; this is done by varying the considered Laplacians. The main ideas of this approach are numerically demonstrated on hypercubic lattices. We restricted our investigation on G_5 and focus on graph homogeneity/non-homogeneity effects on Grover's quantum walk. In upcoming work, we will extend our investigation to effects related to varying d and the location of the target vertex w.

In summary, we observe that the results for larger p resemble those of the complete graphs qualitatively, in particular $\gamma_{opt} \approx \gamma_E$, and the corresponding success probability is well approximated by (25). On the other hand, Grover's optimal times grow exponentially with p in a pattern similar to the graph volume increase in Fig. 6. Choosing smaller p, like $p = 0.4$, leads to a slight improvement in Grover's optimal time compared to the homogeneous case $p = 0.5$. But this improvement does not continue with a further decrease of p as the case $p = 0.1$ in the bottom right panel in Fig. 5 shows.

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Data availability The manuscript has no associated data.

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