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OF SHADOWS AND GAPS IN SPATIAL SEARCH

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Spatial search occurs in a connected graph if a continuous-time quantum walk on the adjacency matrix of the graph, suitably scaled, plus a rank-one perturbation induced by any vertex will unitarily map the principal eigenvector of the graph to the characteristic vector of the vertex. This phenomenon is a natural continuous-time analogue of Grover search. The spatial search is said to be optimal if it occurs with constant fidelity and in time inversely proportional to the shadow of the target vertex on the principal eigenvector. Extending a result of Chakraborty *et al.* (*Physical Review A*, **102**:032214, 2020), we prove a simpler characterization of optimal spatial search. Based on this characterization, we observe that some families of distance-regular graphs, such as Hamming and Grassmann graphs, have optimal spatial search. We also show a matching lower bound on time for spatial search with constant fidelity, which extends a bound due to Farhi and Gutmann for perfect fidelity. Our elementary proofs employ standard tools, such as Weyl inequalities and Cauchy determinant formula.

Keywords: Quantum walk, spatial search, spectral gap, perturbation.

1 Introduction

In the seminal work [1], Grover described a quantum algorithm with a provable quadratic speedup for the ubiquitous search problem. It was realized later that his algorithm can be viewed as a discrete-time quantum walk on the complete graph [2, 3]. In another fundamental work, Farhi and Gutmann [4] proposed a continuous-time analog of Grover search. Their work was generalized by Childs and Goldstone [5] to arbitrary graphs where the problem is known as *spatial search*.

Suppose G is an undirected and connected graph on n vertices with normalized adjacency matrix A whose spectral decomposition is given by $A = \sum_{r=1}^{d} \theta_r E_r$, where $1 = \theta_1 > \theta_2 > \ldots >$

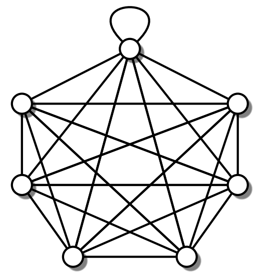

Fig. 1. Grover search in continuous-time (see Farhi and Gutmann [4]): a continuous-time quantum walk with $H = \gamma A(K_n) + e_w e_w^T$ can perfectly transfer the density matrix $E_1 = \frac{1}{n} J_n$ to the target state $e_w e_w^T$, for some $\gamma > 0$, in time $\frac{\pi}{2}\sqrt{n}$. Here, e_w denote the unit vector associated to vertex w of the clique.

$\theta_d \geq 0$ and E_r is the orthogonal projection onto the eigenspace corresponding to θ_r. We say G has optimal spatial search if for any vector w (which may correspond to the characteristic vector of a vertex of G), the continuous-time quantum walk

$$\rho(t) = e^{-itH} \rho(0) e^{itH}$$

with the time-independent Hamiltonian $H = \gamma A + ww^\dagger$, for a scaling factor $\gamma > 0$, maps the density matrix $\rho(0) = E_1$ to the target state $ww^\dagger$ with a constant fidelity, that is,

$$f(t) := \mathrm{Tr}(ww^\dagger \rho(t)) = \Omega_n(1),$$

in time $t = O_n(1/\epsilon_1)$, where $\epsilon_1 = \|E_1 w\|$ is the shadow of the target vertex on the principal eigenspace of G.

Farhi and Gutmann [4] showed that the complete graphs have spatial search (which recovers Grover's result in the continuous-time setting). They also proved a time lower bound of $\Omega_n(\sqrt{n})$ for any continuous-time quantum algorithm with unit fidelity on vertex-transitive graphs. As our first result, we strengthen their time lower bound to $\Omega_n(1/\epsilon_1)$ which holds for constant fidelity (instead of perfect). This lower bound justifies the requirement that the optimal time is $O_n(1/\epsilon_1)$.

Chakraborty *et al.* [6] observed a striking property: a constant spectral gap Δ_2 is sufficient for optimal spatial search. Here, $\Delta_2 = \theta_1 - \theta_2$ is the distance between the two largest normalized eigenvalues of the graph. In particular, this implies that random graphs exhibit spatial search property almost surely. But, this does not explain why the n-cube has spatial search (studied by Childs and Goldstone [5]) since the spectral gap vanishes as n grows.

Subsequently, Chakraborty *et al.* [7] improved the observation from [6] by showing a characterization of optimal spatial search under the assumption of

$$\epsilon_1 \ll \frac{S_1 S_2}{S_3} \quad \text{and} \quad \epsilon_1 \ll \sqrt{S_2}\Delta_2, \tag{1}$$

where $S_k = \sum_{r=2}^{d} \|E_r w\|^2 (\theta_1 - \theta_r)^{-k}$, for $k = 1, 2, 3$, are spectral parameters related to the graph G. Another crucial observation made in [7] is that S_1 is the best choice for the scaling parameter γ. As stated in [7], the unconditional characterization of graphs with optimal spatial search is a longstanding open question.

In this work, we improve the result of Chakraborty *et al.* [7] by showing a characterization of optimal spatial search under the simpler assumption

$$\epsilon_1 \ll \sqrt{S_1}\Delta_2,$$

also under the choice of $\gamma = S_1$. We show that our assumption is asymptotically similar to the second condition in Equation (1) for the relevant ranges of interest. Our improvement is obtained through tighter estimates on the leading eigenvalue perturbations derived from a determinant formula of Cauchy. We also observe a critical condition (hidden in previous analyses) for the strict interlacing between pairs of the two largest eigenvalues of the matrices, before and after perturbation. For this, we explicitly require the second largest eigenvalue of the graph belong to the eigenvalue support of the target vertex, and then appeal to Weyl inequalities to provide strict interlacing.

We then apply the characterization to provide new examples of graphs with optimal spatial search and to offer alternative proofs for existing families. For example, we observe that the Hamming graphs $H(n,q)$, for any constant q, have optimal spatial search. As a special case, this include the binary n-cube $H(n,2)$ which was observed by Childs and Goldstone [5]. For another example, we observe that strongly regular graphs have optimal spatial search since they also have constant spectral gap. This confirms the observation of Janmark *et al.* [8] obtained using degenerate perturbation theory.

For distance regular graphs with larger diameter, Wong [9] and then Tanaka *et al.* [10] proved that the Johnson graphs $J(n,k)$, for constant $k \geq 3$, have spatial search. Since the constant spectral gap condition holds for Johnson graphs, this provides an alternative and immediate proof that they have optimal spatial search. Moreover, we also observe that Grassmann graphs and, in fact, most bounded diameter distance-regular graphs with classical parameters have optimal spatial search (see Figure 2). Both of these are again consequences of the constant spectral gap condition.

Our original motivation for this work was to understand obstructions to optimal spatial search. To this end, we found a collection of necessary conditions for spatial search which are largely based on techniques used in [7]. Aside from being a crucial ingredient for proving the tight characterization, these necessary conditions provide asymptotic explanations why certain families of graphs lack the spatial search property. For example, they can be used to show explicitly why cycles lack optimal spatial search – a well-known folklore result. These conditions can potentially be adapted to other classes such as a small Cartesian product of cycles.

The proofs we employ are elementary as they only use basic tools from matrix theory which do not appeal to perturbative methods. We nevertheless adopt standard asymptotic arguments commonly used in random graphs and complexity of algorithms.

2 Background

We assume the standard inner product $\langle v, w\rangle$ over $\mathbb{C}^n$. All vectors are assumed normalized under the 2-norm defined by $\|w\| = \sqrt{\langle w, w\rangle}$. The set of all $n \times n$ matrices with complex entries is denoted $\mathrm{Mat}_n(\mathbb{C})$. As with vectors, we define the 2-norm of a matrix as $\|A\| = \sqrt{\langle A, A\rangle}$, where $\langle A, B\rangle = \mathrm{Tr}(A^\dagger B)$ is the inner product between matrices. The spectrum $\mathrm{Spec}(A)$ of a matrix A is the set of its eigenvalues. In this work, we will focus primarily on Hermitian matrices whose eigenvalues are guaranteed to be real. We adopt the notation $\lambda_i(A)$ to represent the ith largest eigenvalue of the matrix A. We call a Hermitian matrix *normalized* if its spectrum lies in $[0, 1]$ *and* 1 is a simple eigenvalue; so, in this case $1 = \lambda_1(A) > \lambda_2(A) \geq \ldots \geq \lambda_n(A) \geq 0$.

In stating the spectral decomposition of a Hermitian matrix, say $A = \sum_{r=1}^{d} \theta_r E_r$, we always assume the distinct eigenvalues are listed in decreasing order, that is, $\theta_1 > \theta_2 > \ldots > \theta_d$. Recall that E_r is the orthogonal projection onto the eigenspace corresponding to eigenvalue θ_r where E_r is Hermitian with $E_r^2 = E_r$, $\sum_{r=1}^{d} E_r = I$, and $E_r E_s = E_r$ if $r = s$ and is 0 otherwise. The *eigenvalue support* of a vector $w \in \mathbb{C}^n$ with respect to A is defined as

$$\mathrm{Supp}_A(w) = \{\theta_r : \|E_r w\| \neq 0\}, \tag{2}$$

which is the set of eigenvalues whose eigenspaces are not fully contained in the subspace $w^\perp$. For each positive integer k, we let

$$S_k = \sum_{r=2}^{d} \frac{\|E_r w\|^2}{(\theta_1 - \theta_r)^k}. \tag{3}$$

These are spectral parameters which will play an important role in characterizing optimal spatial search. They originally appeared in Childs and Goldstone [5]. Further background on matrix theory may be found in Horn and Johnson [11].

Asymptotics We use the standard asymptotic notation to compare the relative order of magnitude of two sequences of numbers f_n and g_n depending on a parameter $n \to \infty$. Our main source is Janson *et al.* [12]. We assume $f_n, g_n > 0$ for sufficiently large n. We write:

- $f_n \lesssim g_n$ or $f_n = O_n(g_n)$ as $n \to \infty$ if there exist constants $c, n_0 > 0$ such that $f_n \leq c g_n$ for $n \geq n_0$.
- $f_n \gtrsim g_n$ or $f_n = \Omega_n(g_n)$ as $n \to \infty$ if there exist constants $c, n_0 > 0$ such that $f_n \geq c g_n$ for $n \geq n_0$.
- $f_n \asymp g_n$ or $f_n = \Theta_n(g_n)$ as $n \to \infty$ if $f_n = O_n(g_n)$ and $f_n = \Omega_n(g_n)$.
- $f_n \ll g_n$ or $f_n = o_n(g_n)$ if $f_n / g_n \to 0$ as $n \to \infty$.
- $f_n \gg g_n$ or $f_n = \omega_n(g_n)$ if $g_n / f_n \to 0$ as $n \to \infty$.
- $f_n \sim g_n$ if $f_n / g_n \to 1$ as $n \to \infty$.

We omit the expression "as $n \to \infty$" when it is clear from context. Given that most results are asymptotic, we assume that n is sufficiently large without explicitly stating this.

Our focus is on a family of graphs $\{G_n\}_{n=1}^{\infty}$ instead of individual graphs, and hence most assertions are asymptotic in nature and will depend on n as it tends to ∞. When it is clear, we simply write G_n for the family of graphs, and even simply G if n is understood from context. Given a graph $G = (V, E)$ that is undirected, its adjacency matrix $A(G)$ is a matrix whose (u, v)-entry is 1 if $(u, v) \in E$, and is 0 otherwise. In this work, we will allow the adjacency matrix be a Hermitian matrix whose nonzero entries are complex valued, and will denote it as $H(G)$. For example, this may include the case of signed graphs (± 1 entries) or complex oriented graphs ($\pm i$ entries).

A continuous-time quantum walk on G with a Hermitian adjacency matrix $H(G)$ is governed by the Schrödinger equation defined by

$$\rho'(t) = -i[H(G), \rho(t)] \tag{4}$$

where $\rho(t)$ is a positive semidefinite matrix of unit trace (also called a density matrix). Here, $[A, B] = AB - BA$ denotes the commutator of two matrices $A, B \in \mathrm{Mat}_n(\mathbb{C})$. The solution of the above equation is given by

$$\rho(t) = e^{-itH(G)}\rho(0)e^{itH(G)}.$$

We adopt the density matrix formulation of the Schrödinger evolution since it leads to simpler analyses overall (as global phase factors disappear, for example) and it can be easily generalized to more realistic settings. For more background on quantum information, please see Nielsen and Chuang [13]

Given that spatial search is heavily influenced by the seminal work [1], in the rest of this paper we will call a graph with the optimal spatial search property *Groverian.*

Definition 1 *Let $\{G_n\}$ be a family of graphs with normalized adjacency matrix $H(G_n)$ where E_1 is the orthogonal projection onto its principal eigenspace. We say G_n is γ-*Groverian *if for any $w \in \mathbb{C}^n$ with $\|E_1 w\| \neq 0$, the density matrix evolution defined by*

$$\rho(t) = U(t)\rho(0)U(t)^{-1}, \qquad \text{with } \rho(0) = E_1,$$

where $U(t) = \exp(-it(\gamma H(G_n) + ww^\dagger))$, there is a time $\tau = O_n(1/\|E_1 w\|)$ so that the fidelity satisfies

$$f(\tau) := \mathrm{Tr}(ww^\dagger \rho(\tau)) = \Omega_n(1). \tag{5}$$

The family of graphs is Groverian if it is γ-Groverian for some $\gamma > 0$.

The condition on time is the *quadratic speedup* requirement that is the hallmark signature of Grover search. This is because the probability of measuring w given the state E_1 is $\|E_1 w\|^2$, and hence generating w has a geometric time of $1/\|E_1 w\|^2$.

For a spatial search algorithm to be fully constructive, most previous works require the graphs be vertex transitive. This assumption was made in Farhi and Gutmann [4] and in Childs and Goldstone [5]. This guarantees that the choice of the scaling parameter γ and the time t in Definition 1 are not dependent on the vertex w. But, as pointed out by Meyer and Wong [14], we can also allow graphs whose automorphism group has a constant number of orbits. They observed that the search algorithm can simply check each orbit separately as most of the relevant spectral parameters are constant within each orbit.[a] Note that a vertex transitive graph has only a single orbit. In this work, we will place the same assumption on our graphs.

Given that most of our statements hold for Hermitian matrices, we will view graphs largely through their Hermitian adjacency matrices. To that end, we fix a convenient terminology to capture a triplet of a Hermitian matrix, a unit norm vector and a positive scalar that will play a central role in all of our assertions.

[a] A pertinent example given in [14] is the *barbell* graph obtained from connecting two disjoint cliques K_n by a single edge; this graph has two orbits with sizes 2 and $2n - 2$, respectively.

Assumption 2 *We call (H, w, γ) a* tuplet *if the following (notational) assumptions hold.*

(a) $H \in \mathrm{Mat}_n(\mathbb{C})$ *is a normalized Hermitian matrix whose spectral decomposition is* $H = \sum_r \theta_r E_r$. *Recall that as H is normalized, its eigenvalues lie in $[0,1]$ and 1 is a simple eigenvalue.*

(b) $w \in \mathbb{C}^n$ *is a vector with unit norm which satisfies* $\|E_1 w\| \neq 0$ *and* $\|E_1 w\| = o_n(1)$. *Whenever it is clear from context, we will use the abbreviated notation* $\epsilon_1 := \|E_1 w\|$.

(c) $\gamma \in \mathbb{R}$ *is a positive scalar whereby the perturbed matrix* $\gamma H + ww^\dagger$ *has the spectral decomposition* $\sum_p \zeta_p F_p$.

3 Time Lower Bounds

We motivate the condition on time in Definition 1. Farhi and Gutmann [4] proved that spatial search with fidelity 1 on a vertex-transitive graph requires time $\Omega_n(\sqrt{n})$. We extend their result to show a time lower bound of $\Omega_n(1/\epsilon_1)$ for constant fidelity which applies to arbitrary graphs. Note that $\epsilon_1 = 1/\sqrt{n}$ for vertex-transitive graphs whenever w denote the characteristic vector of a vertex. This matching lower bound justifies the choice of the optimal time.

Theorem 1 *Let (H, w, γ) be a tuplet where H is γ-Groverian at time τ. Then,* $\tau = \Omega_n(1/\epsilon_1)$.

Proof. The first part of the proof follows [4] but in the density matrix language. Let $H_w = H_0 + ww^\dagger$, where $H_0 = \gamma H$. We compare two density matrix evolutions given by

$$\rho_w'(t) = -i[H_w, \rho_w(t)], \quad \rho_0'(t) = -i[H_0, \rho_0(t)] \tag{6}$$

with $\rho_w(0) = \rho_0(0) = E_1$. Note $\rho_0(t) = E_1$ for all t. Assume for now that the fidelity is one or $\rho_w(\tau) = ww^\dagger$. We will remove this assumption later.

The proof proceeds by analyzing bounds on $\|\rho_w(t) - \rho_0(t)\|^2$. First, by taking derivative, we have

$$\frac{d}{dt}\|\rho_w(t) - \rho_0(t)\|^2 = -2\langle \rho_w(t), \rho_0(t)\rangle'.$$

From the product rule and Equation (6), we see that

$$\begin{aligned}
\langle \rho_w(t), \rho_0(t)\rangle' &= \langle \rho_w(t), \rho_0'(t)\rangle + \langle \rho_w'(t), \rho_0(t)\rangle \\
&= i\langle [H_w, \rho_w(t)], E_1\rangle \\
&= i\langle w, [E_1, \rho_w(t)]w\rangle.
\end{aligned}$$

Now, notice that

$$\begin{aligned}
|\langle w, [E_1, \rho_w(t)]w\rangle| &\leq 2|\langle w, E_1\rho_w(t)w\rangle|, \quad \text{as } |x^\dagger[A,B]x| \leq 2|x^\dagger(AB)x| \\
&\leq 2\|E_1 w\|\,\|\rho_w(t)w\|, \quad \text{since } |\langle a, b\rangle| \leq \|a\|\,\|b\| \\
&\leq 2\epsilon_1, \qquad \text{because } \|\rho_w(t)w\| \leq 1.
\end{aligned}$$

Putting these together, we get

$$\left|\frac{d}{dt}\|\rho_w(t) - \rho_0(t)\|^2\right| \;\leq\; 4\epsilon_1.$$

By the Fundamental Theorem of Calculus, we obtain

$$\|\rho_w(\tau) - \rho_0(\tau)\|^2 \;=\; \int_0^\tau \left(\frac{d}{dt}\|\rho_w(t) - \rho_0(t)\|^2\right) dt \;\leq\; 4\epsilon_1\tau. \tag{7}$$

Since $\rho_w(\tau) = ww^\dagger$, we have $\|\rho_w(\tau) - \rho_0(\tau)\|^2 = 2(1 - \epsilon_1^2)$, and therefore

$$1 - \epsilon_1^2 \;\leq\; 2\epsilon_1\tau,$$

which yields the lower bound $\tau = \Omega_n(1/\epsilon_1)$.

Finally, we remove the assumption $\rho_w(\tau) = ww^\dagger$. Suppose that $\left\|\rho_w(\tau) - ww^\dagger\right\|^2 \leq \delta$, for some $\delta \in (0,1)$. Our strategy is to reduce this case to the former case by using the following inequality.

Fact 2 *(Triangle Inequality for Squared Norm) For matrices $A, B, C \in \mathrm{Mat}_n(\mathbb{C})$,*

$$\|A - C\|^2 \leq 2\|A - B\|^2 + 2\|B - C\|^2.$$

Proof. Squaring the triangle inequality, we get

$$\|A - C\|^2 \leq \|A - B\|^2 + \|B - C\|^2 + 2\|A - B\|\,\|B - C\|.$$

Now, observe $0 \leq (\|A - C\| - \|B - C\|)^2$. □

Applying Fact 2, we see that

$$2\|\rho_w(\tau) - \rho_0(\tau)\|^2 \geq \left\|ww^\dagger - \rho_0(\tau)\right\|^2 - 2\left\|\rho_w(\tau) - ww^\dagger\right\|^2 \geq \left\|ww^\dagger - \rho_0(\tau)\right\|^2 - 2\delta.$$

Thus, we have

$$\|\rho_w(\tau) - \rho_0(\tau)\|^2 \;\geq\; (1 - \epsilon_1^2 - \delta)$$

which can be combined with Equation (7) to obtain $\tau = \Omega_n(1/\epsilon_1)$. □

4 Interlacing

We review some relevant tools from matrix theory and prove a few preliminary results.

4.1 Weyl Inequalities

A theorem of Weyl on eigenvalue interlacing is key to our analysis. Given that we restate the theorem slightly, we prove it for completeness.

Lemma 1 *(Subspace intersection, Lemma 4.2.3 in [11])*
Let $W_1, \ldots, W_k$ be subspaces of $\mathbb{C}^n$ and let $d = \dim W_1 + \ldots + \dim W_k - (k-1)n$. If $d \geq 1$, then $\dim(\bigcap_{i=1}^k W_i) \geq d$. In particular, there is a unit vector in $W_1 \cap \ldots \cap W_k$.

Proof. Note that $\dim(W_1 \cap W_2) + \dim(W_1 + W_2) = \dim W_1 + \dim W_2$, which implies $\dim(W_1 \cap W_2) \geq \dim W_1 + \dim W_2 - n$. So, if $\dim W_1 + \dim W_2 - n \geq 1$, then $W_1 \cap W_2$ contains a nonzero vector. The claim follows by induction. □

Theorem 3 *(Weyl Interlacing, restatement of Lemma 4.3.1 in [11])*
Let A, B be two $n \times n$ Hermitian matrices. For $i = 1, \ldots, n$, we have

$$\lambda_i(A+B) \;\leq\; \lambda_{i-j}(A) + \lambda_{j+1}(B), \quad j = 0, \ldots, i-1 \tag{8}$$

with equality if and only if there is $v \neq 0$ so that $(A+B)v = \lambda_i(A+B)v$, $Av = \lambda_{i-j}(A)v$, and $Bv = \lambda_{j+1}(B)v$, and we have

$$\lambda_{i+j}(A) + \lambda_{n-j}(B) \;\leq\; \lambda_i(A+B), \quad j = 0, \ldots, n-i \tag{9}$$

with equality if and only if there is $v \neq 0$ so that $(A+B)v = \lambda_i(A+B)v$, $Av = \lambda_{i+j}(A)v$, and $Bv = \lambda_{n-j}(B)v$.

Proof. For $i = 1, \ldots, n$, let z_i, x_i, and y_i be orthonormal eigenvectors of A, B, and $A+B$, respectively, corresponding to their ith largest eigenvalues.

We define $W_1 = \text{span}\{z_{i-j}, \ldots, z_n\}$, $W_2 = \text{span}\{x_{j+1}, \ldots, x_n\}$, and $W_3 = \text{span}\{y_1, \ldots, y_i\}$. Let $d_1 = \dim W_1 = n - i + j + 1$, $d_2 = \dim W_2 = n - j$, and $d_3 = \dim W_3 = i$. Since $\dim(W_1 \cap W_2 \cap W_3) = d_1 + d_2 + d_3 - \dim(W_1 + W_2 + W_3) \geq d_1 + d_2 + d_3 - 2n = 1$, the subspace $W_1 \cap W_2 \cap W_3$ contains a nonzero vector v. For any nonzero $v \in W_1 \cap W_2 \cap W_3$, we have

$$\lambda_i(A+B) \leq v^\dagger(A+B)v \leq \lambda_{i-j}(A) + \lambda_{j+1}(B), \quad \text{for } j = 0, \ldots, i-1. \tag{10}$$

Equality is achieved for i, j if and only if there is a nonzero $v \in W_1 \cap W_2 \cap W_3$ for which $(A+B)v = \lambda_i(A+B)v$, $Av = \lambda_{i-j}(A)v$, and $Bv = \lambda_{j+1}(B)v$.

For the second inequality, observe that $\lambda_i(-A) = -\lambda_{n-i+1}(A)$. Therefore,

$$-\lambda_{n-i+1}(A+B) = \lambda_i(-A-B) \leq \lambda_{i-j}(-A) + \lambda_{j+1}(-B) = -\lambda_{n-i+j+1}(A) - \lambda_{n-j}(B) \tag{11}$$

which implies

$$\lambda_{n-i+j+1}(A) + \lambda_{n-j}(B) \leq \lambda_{n-i+1}(A+B). \tag{12}$$

Now, rename $n-i+1$ to i and keep j (and hence $n-i+j+1$ to $i+j$). This yields

$$\lambda_{i+j}(A) + \lambda_{n-j}(B) \leq \lambda_i(A+B), \quad \text{for } j = 0, \ldots, n-i. \tag{13}$$

Equality is achieved for i, j if and only if there is a nonzero $v \in W_1 \cap W_2 \cap W_3$ for which $(A+B)v = \lambda_i(A+B)v$, $Av = \lambda_{i+j}(A)v$, and $Bv = \lambda_{n-j}(B)v$ with $W_1 = \text{span}\{z_1, \ldots, z_{i+j}\}$, $W_2 = \text{span}\{x_1, \ldots, x_{n-j}\}$, and $W_3 = \text{span}\{y_i, \ldots, y_n\}$. □

Lemma 2 *(Strict Interlacing) Let H be a normalized $n \times n$ Hermitian matrix with spectral decomposition $H = \sum_r \theta_r E_r$. Let $w \in \mathbb{C}^n$ be a vector with unit norm where $\theta_1, \theta_2 \in \text{Supp}_H(w)$. Then for any $\gamma > 0$, the two largest eigenvalues of $\gamma H + ww^\dagger$ are simple and they strictly interlace the two largest eigenvalues of γH.*

Proof. We apply Theorem 3 with $A = \gamma H$ and $B = ww^\dagger$. Note $\lambda_1(H) = \lambda_1(ww^\dagger) = 1$ are simple eigenvalues, and $\lambda_j(ww^\dagger) = 0$ for $j = 2, \ldots, n$. From Equation (9), with $i = 1$ and $j = 0$, we get

$$\lambda_1(\gamma H) + \lambda_n(ww^\dagger) = \lambda_1(\gamma H) \leq \lambda_1(\gamma H + ww^\dagger). \tag{14}$$

Similarly, from Equation (8), with $i = 2$ and $j = 1$, we get

$$\lambda_2(\gamma H + ww^\dagger) \leq \lambda_1(\gamma H) + \lambda_2(ww^\dagger) = \lambda_1(\gamma H). \tag{15}$$

Both of the inequalities above are strict since $\lambda_1(H)$ is simple and $E_1 w \neq 0$ implies $ww^\dagger z_1 \neq 0$ where z_1 is the principal eigenvector with $z_1 z_1{}^\dagger = E_1$.

Next, we apply Theorem 3 with $i = 2$ and $j = 0$ in Equation (9), to get

$$\lambda_2(\gamma H) + \lambda_n(ww^\dagger) = \lambda_2(\gamma H) \leq \lambda_2(\gamma H + ww^\dagger). \tag{16}$$

Since $\theta_2 \in \mathrm{Supp}_H(w)$, there exists an eigenvector z_2 corresponding to $\lambda_2(H)$ so that $ww^\dagger z_2 \neq 0$. For any nonzero vector v from the subspace $W_1 \cap W_2 \cap W_3$ (as constructed in the proof of Theorem 3), with $W_1 = \mathrm{span}\{z_1, z_2\}$, we always have $ww^\dagger z_2 \neq 0$ and hence the inequality in Equation (16) is strict. □

4.2 Cauchy's Equality

The next formula due to Cauchy can be derived from the determinant of bordered matrices (see [11]).

Lemma 3 *(Cauchy) For any $n \times n$ matrix A, any vectors $x, y \in \mathbb{C}^n$, we have*

$$\det(A + xy^\dagger) = \det(A) + y^\dagger \,\mathrm{Adj}(A) x. \tag{17}$$

Moreover, if A is nonsingular, then

$$\det(A + xy^\dagger) = \det(A)(1 + y^\dagger A^{-1} x). \tag{18}$$

We apply the above lemma to provide sharper estimates for the case when $\gamma = S_1$ on the locations of the two largest perturbed eigenvalues relative to the unperturbed principal eigenvalue.

Proposition 4 *Let (H, w, S_1) be a tuplet. Then*

$$\epsilon_1^2 \;<\; \zeta_1 - S_1 \;\lesssim\; \sqrt{S_1}\epsilon_1. \tag{19}$$

Moreover, if $\theta_2 \in \mathrm{Supp}_H(w)$, then

$$0 \;<\; S_1 - \zeta_2 \;\lesssim\; \sqrt{S_1}\epsilon_1. \tag{20}$$

Proof. Let $\tilde{H} = S_1 H + ww^\dagger$ and $\Delta_r = 1 - \theta_r$, for all r. Note that $\phi(\tilde{H}, t) = \det((tI - S_1 H) - ww^\dagger)$. Applying Lemma 3 and assuming m_r is the multiplicity of θ_r, we get

$$\begin{aligned} \phi(\tilde{H}, t) &= \det(tI - S_1 H)(1 - w^\dagger (tI - S_1 H)^{-1} w) \\ &= \left(\prod_r (t - S_1\theta_r)^{m_r}\right)\left(1 - \sum_r \frac{\|E_r w\|^2}{(t - S_1\theta_r)}\right). \end{aligned}$$

The bound $\zeta_1 - S_1 > \epsilon_1^2$ follows by verifying that $\phi(\tilde{H}, S_1 + \epsilon_1^2)$ is negative. Observe that if $\phi(\tilde{H}, S_1 + \beta) > 0$, then $\zeta_1 - S_1 \leq \beta$. We write the condition $\phi(\tilde{H}, S_1 + \beta) > 0$ as

$$1 \;>\; \sum_r \frac{\|E_r w\|^2}{S_1\Delta_r + \beta} \;=\; \frac{\epsilon_1^2}{\beta} + \sum_{r\neq 1} \frac{\|E_r w\|^2}{S_1\Delta_r + \beta}.$$

Because $\Delta_r \leq 1$, for each r, it follows that $(1+\beta/S_1)^{-1}$ is an upper bound for the sum $\sum_{r\neq 1} \|E_r w\|^2/(S_1\Delta_r + \beta)$. So, to satisfy the previous inequality, it suffices to require

$$1 \;>\; \frac{\epsilon_1^2}{\beta} + \frac{1}{1+\beta/S_1}.$$

After straightforward calculations, we obtain $\beta^2 - \epsilon_1^2\beta - S_1\epsilon_1^2 > 0$. The roots of this quadratic equation are given by

$$\beta_{\pm} = \frac{1}{2}(\epsilon_1^2 \pm \sqrt{\epsilon_1^4 + 4S_1\epsilon_1^2}).$$

The positive root is given by $\beta_+ = O_n(\sqrt{S_1}\epsilon_1)$, since $\epsilon_1 \ll 1$, which proves Equation (19).

We denote $\delta_- = \zeta_2 - S_1$. By Lemma 2, $|\delta_-| > 0$. Now, observe that if $\phi(\tilde{H}, S_1 - \beta) > 0$ then $|\delta_-| \leq \beta$. As above, we write the condition $\phi(\tilde{H}, S_1 - \beta) > 0$ as

$$1 \;<\; \sum_r \frac{\|E_r w\|^2}{S_1\Delta_r - \beta} \;=\; -\frac{\epsilon_1^2}{\beta} + \sum_{r\neq 1} \frac{\|E_r w\|^2}{S_1\Delta_r - \beta}.$$

This yields

$$\sum_{r\neq 1} \frac{\|E_r w\|^2}{S_1\Delta_r} \frac{1}{1-\beta/(S_1\Delta_r)} \;>\; 1 + \frac{\epsilon_1^2}{\beta}.$$

As $\Delta_r \leq 1$, for $r \geq 2$, we note that $1/(1-\beta/S_1)$ is a lower bound for the expression on the left-hand side. Therefore, we may require instead

$$\frac{1}{1-\beta/S_1} \;>\; 1 + \frac{\epsilon_1^2}{\beta}$$

which simplifies to $\beta^2 + \epsilon_1^2\beta - S_1\epsilon_1^2 \;>\; 0$. The maximum root of the quadratic polynomial is given by

$$\beta = \frac{1}{2}(-\epsilon_1^2 + \sqrt{\epsilon_1^4 + 4S_1\epsilon_1^2}) \;\sim\; \sqrt{S_1}\epsilon_1$$

which proves Equation (20). □

5 Necessary Gaps

We describe necessary conditions for graphs to be Groverian, but first we derive some useful preliminary observations. Our analysis borrows heavily ideas from Chakraborty *et al.* [7].

We start by restating the machinery in [7] (specifically, Theorem 4) using our notation for the sake of consistency and to point out certain explicit assumptions that are required. Given a tuplet (H, w, γ), for each p, we have $(\gamma H + ww^\dagger)F_p = \zeta_p F_p$ or

$$ww^\dagger F_p = (\zeta_p I - \gamma H)F_p, \tag{21}$$

which implies

$$\|F_p w\|^2 w = (\zeta_p I - \gamma H)F_p w. \tag{22}$$

If $\zeta_p \notin \mathrm{Spec}(\gamma H)$ holds, it clearly guarantees

$$\frac{F_p w}{\|F_p w\|^2} = (\zeta_p I - \gamma H)^{-1} w, \tag{23}$$

which further yields

$$\frac{1}{\|F_p w\|^2} = \sum_r \frac{\|E_r w\|^2}{(\zeta_p - \gamma\theta_r)^2}. \tag{24}$$

Moreover, Equation (23) yields an expression of unity

$$1 = \sum_{r=1}^{d} \frac{\|E_r w\|^2}{\zeta_p - \gamma\theta_r}. \tag{25}$$

Returning to Equation (22), after multiplying both sides by E_1, we derive

$$\|F_p w\|^2 E_1 w = (\zeta_p - \gamma) E_1 F_p w. \tag{26}$$

By Theorem 3, since $\|E_1 w\| \neq 0$, we have strict interlacing where $\zeta_2 < \gamma < \zeta_1$. Furthermore, $\gamma \neq \zeta_r$, for all $r = 1, \ldots, n$. This allows us to write

$$E_1 F_p w \;=\; \frac{\|F_p w\|^2}{\zeta_p - \gamma} E_1 w, \qquad p = 1, \ldots, m. \tag{27}$$

Now, analyzing the fidelity of the quantum walk with the Hamiltonian $\tilde{H} = \gamma H + ww^\dagger$, we get

$$f(t) \;=\; \mathrm{Tr}(ww^\dagger e^{-it\tilde{H}} E_1 e^{it\tilde{H}}) \;=\; \sum_{p,q} e^{-it(\zeta_p - \zeta_q)} w^\dagger F_p E_1 F_q w. \tag{28}$$

After expanding $w^\dagger F_p E_1 F_q w$ to $(w^\dagger F_p E_1)(E_1 F_q w)$ since $E_1^2 = E_1$, we use Equation (27) to substitute $E_1 F_q w$ and $(E_1 F_p w)^\dagger$ to get

$$f(t) \;=\; \sum_p e^{-it\zeta_p} \frac{\|F_p w\|^2}{\zeta_p - \gamma} \sum_q e^{it\zeta_q} \frac{\|F_q w\|^2}{\zeta_q - \gamma} \|E_1 w\|^2$$

since $(w^\dagger E_1)(E_1 w) = \|E_1 w\|^2$. Thus,

$$f(t) \;=\; \epsilon_1^2 \left| \sum_p e^{-it\zeta_p} \frac{\|F_p w\|^2}{(\zeta_p - \gamma)} \right|^2. \tag{29}$$

By triangle inequality, the above becomes

$$f(t) \;\leq\; \epsilon_1^2 \left(\sum_p \frac{\|F_p w\|^2}{|\zeta_p - \gamma|} \right)^2. \tag{30}$$

Finally, from Equation (29) at the time of origin $t = 0$, we get another expression of unity,

$$1 \;=\; \left| \frac{\|F_1 w\|^2}{\zeta_1 - \gamma} - \sum_{p \geq 2} \frac{\|F_p w\|^2}{\gamma - \zeta_p} \right| \tag{31}$$

since the first term $\|F_1 w\|^2 / (\zeta_1 - \gamma)$ and the subsequent terms $\|F_p w\|^2 / (\zeta_p - \gamma)$, for $p \geq 2$, differ in sign because $\zeta_1 > \gamma > \zeta_p$. As $|A - B| \geq |A| - |B|$ by triangle inequality, the last equation immediately implies the following pair of inequalities:

$$\sum_{p \geq 2} \frac{\|F_p w\|^2}{\gamma - \zeta_p} \leq \frac{\|F_1 w\|^2}{\zeta_1 - \gamma} + 1, \quad \frac{\|F_1 w\|^2}{\zeta_1 - \gamma} \leq \sum_{p \geq 2} \frac{\|F_p w\|^2}{\gamma - \zeta_p} + 1. \tag{32}$$

Using the above, we are ready to observe some necessary conditions for a graph G to be Groverian. In the next theorem, we show some conditions on ϵ_1 in relation to the eigenvalue gaps between the largest unperturbed eigenvalue of $\gamma H(G)$ and the perturbed eigenvalues ζ_m of $\gamma H(G) + ww^\dagger$. In particular, for a graph G to be Groverian, ϵ_1 must be asymptotically equal to the first gap $\delta_+ := \zeta_1 - \gamma$, it must be asymptotically greater or equal to the second gap $\delta_- := \gamma - \zeta_2$, and it must be asymptotically equal to some gap $\gamma - \zeta_p$, for some $p \geq 2$, but not necessarily the second gap. Recall that by strict interlacing, we know that $\gamma\theta_2 < \zeta_2 < \gamma < \zeta_1$, where θ_2 is the second largest eigenvalue of $H(G)$.

The first two observations in the following theorem are implicit in the proof of Theorem 4 in [7] but it will be useful to restate them in our notation below. The third observation appears to be new.

Theorem 5 *For a tuplet (H, w, γ), suppose one of the following conditions holds:*

(i) $\epsilon_1 \not\asymp \zeta_1 - \gamma$ (equivalently, $\epsilon_1 \ll \zeta_1 - \gamma$ or $\epsilon_1 \gg \zeta_1 - \gamma$), or

(ii) $\epsilon_1 \ll \gamma - \zeta_2$, or

(iii) $\gamma - \zeta_{p-1} \ll \epsilon_1 \ll \gamma - \zeta_p$, for some $p \geq 3$.

Then, H is not γ-Groverian.

Proof. We treat each condition as a separate case.

Case (i): Denote $\delta_+ := \zeta_1 - \gamma$ and assume that $\delta_+ \not\asymp \epsilon_1$. From Equation (30), we apply Equation (32) to obtain the following upper bound

$$f(t) \;\leq\; \epsilon_1^2 \left(\frac{2\left\|F_1 w\right\|^2}{\delta_+} + 1 \right)^2 \;=\; \left(2\frac{\epsilon_1}{\delta_+}\left\|F_1 w\right\|^2 + \epsilon_1 \right)^2, \tag{33}$$

which shows that fidelity goes to zero if $\epsilon_1 \ll \delta_+$. For the opposite direction, apply Equation (24) with $p = 1$ to get

$$\frac{1}{\left\|F_1 w\right\|^2} \;=\; \sum_{r=1}^{d} \frac{\left\|E_r w\right\|^2}{(\zeta_1 - \gamma\theta_r)^2}.$$

But, the sum is bounded from below by its first term, and so $\left\|F_1 w\right\|^2 \leq \delta_+^2/\epsilon_1^2$. Returning to Equation (33) and using the preceding upper bound,

$$f(t) \leq \left(\frac{2\delta_+}{\epsilon_1} + \epsilon_1 \right)^2, \tag{34}$$

which shows that fidelity goes to zero if $\delta_+ \ll \epsilon_1$.

Case (ii): Let $\delta_- := \zeta_2 - \gamma$. We start with Equation (30) and use Equation (31) to rewrite a term in the upper bound as

$$\sum_{p} \frac{\left\|F_p w\right\|^2}{|\gamma - \zeta_p|} \;\leq\; 1 + 2\sum_{p\geq 2} \frac{\left\|F_p w\right\|^2}{\gamma - \zeta_p} \;\leq\; 1 + 2\frac{(1 - \left\|F_1 w\right\|^2)}{|\delta_-|}, \tag{35}$$

since $|\delta_-| \leq \gamma - \zeta_p$ for each $p \geq 2$. Thus, we derive an upper bound on the fidelity,

$$f(t) \leq \left(\frac{2\epsilon_1}{|\delta_-|}(1 - \|F_1 w\|^2) + \epsilon_1\right)^2, \tag{36}$$

which shows that fidelity tends to zero if $\epsilon_1 \ll |\delta_-|$.

Case (iii): Starting with Equation (21), after multiplying by E_1, we derive

$$E_1 w w^\dagger F_p = (\zeta_p - \gamma) E_1 F_p.$$

Taking a product with itself but for index q, we get

$$\epsilon_1^2 F_q w w^\dagger F_p = (\zeta_q - \gamma)(\zeta_p - \gamma) F_q E_1 F_p.$$

Upon taking the trace, this yields

$$\epsilon_1^2 \|F_p w\|^2 = (\zeta_p - \gamma)^2 \langle F_p, E_1 \rangle. \tag{37}$$

By Equation (28), we have

$$\sum_{p,q} e^{-it(\zeta_p - \zeta_q)} w^\dagger F_p E_1 F_q w = \sum_{p,q} e^{-it(\zeta_p - \zeta_q)} \frac{\epsilon_1}{(\zeta_p - \gamma)} \frac{\epsilon_1}{(\zeta_q - \gamma)} \|F_p w\|^2 \|F_q w\|^2,$$

where we have used Equation (27) twice (for both p and q). Now, note we may apply Equation (37) to "flip" one of the ratios as follows:

$$\sum_{p,q} e^{-it(\zeta_p - \zeta_q)} \frac{\epsilon_1}{\zeta_p - \gamma} \frac{\zeta_q - \gamma}{\epsilon_1} \|F_p w\|^2 \langle F_q, E_1 \rangle.$$

This allows us to partition the sums around m based on whether $\epsilon_1 \ll \zeta_p - \gamma$ or $\epsilon_1 \gg \zeta_p - \gamma$. In all cases, the corresponding terms tend to 0 as $n \to \infty$. □

5.1 Failure around S_1

We describe necessary conditions on γ relative to S_1. First, we show failure whenever γ is too large relative to S_1 (which is an alternate restatement of the first half of Theorem 4 in [7]).

Theorem 6 *For a tuplet (H, w, γ), if $\epsilon_1 S_1 \ll \gamma - S_1$, then H is not γ-Groverian.*

Proof. Starting with Equation (25) with $p = 1$, we see

$$1 \;=\; \sum_{r=1}^{d} \frac{\|E_r w\|^2}{\zeta_1 - \gamma\theta_r} \;=\; \frac{\epsilon_1^2}{\delta_+} + \sum_{r=2}^{d} \frac{\|E_r w\|^2}{\gamma(1-\theta_r) + \delta_+} \;\leq\; \frac{\epsilon_1^2}{\delta_+} + \frac{S_1}{\gamma}.$$

After minor rearrangements, we obtain

$$\delta_+ \;\leq\; \epsilon_1^2 \frac{\gamma}{\gamma - S_1} \;=\; \epsilon_1^2 \left(1 + \frac{S_1}{\gamma - S_1}\right) \;\ll\; \epsilon_1(1 + o_n(1)) \tag{38}$$

which proves the claim by appealing to Theorem 5, case *(i)*. □

Next, we show failure conditions when γ is centered around S_1. We will use this later to show that cycles are not Groverian.

Theorem 7 *Let (H, w, γ) be a tuplet where there is a constant $c > 0$ so that $\|E_r w\| \leq c\epsilon_1$, for all $r \geq 2$. Let*

$$I_\alpha = \{r \geq 2 : \gamma < \epsilon_1^\alpha (1 - \theta_r)^{-1}\}.$$

If $\gamma = S_1(1 + o_n(1))$ and $|I_\alpha| \geq 2c^2$, for some $\alpha \in (1, 2)$, then H is not γ-Groverian.

Proof. By Theorem 5, it suffices to show $\delta_+ \ll \epsilon_1$, where $\delta_+ = \zeta_1 - \gamma$. Let $\Delta_r = 1 - \theta_r$. Our plan is to prove $\delta_+ = O_n(\epsilon_1^\alpha)$ for the given $\alpha \in (1, 2)$. By Lemma 3, it is enough to show $\phi(H, \gamma + \epsilon_1^\alpha) > 0$ or equivalently

$$1 \ > \ \sum_{r=1}^{d} \frac{\|E_r w\|^2}{\gamma \Delta_r + \epsilon_1^\alpha} \ = \ \epsilon_1^{2-\alpha} + \frac{1}{\gamma} \sum_{r \geq 2} \frac{\|E_r w\|^2}{\Delta_r + (\epsilon_1^\alpha / \gamma)}.$$

Let us focus on the last summation. After splitting the summation into two parts, we may bound each part from above as follows,

$$\sum_{r \geq 2} \frac{\|E_r w\|^2}{\Delta_r + (\epsilon_1^\alpha / \gamma)} \leq \sum_{\substack{r \geq 2: \\ \Delta_r < \epsilon_1^\alpha / \gamma}} \frac{\|E_r w\|^2}{2\Delta_r} + \sum_{\substack{r \geq 2: \\ \Delta_r \geq \epsilon_1^\alpha / \gamma}} \frac{\|E_r w\|^2}{\Delta_r}.$$

So, to prove the claim, it suffices to show that

$$1 \ > \ \epsilon_1^{2-\alpha} + \frac{1}{\gamma} \sum_{r \geq 2} \frac{\|E_r w\|^2}{\Delta_r} - \frac{1}{2\gamma} \sum_{\substack{r \geq 2: \\ \Delta_r < \epsilon_1^\alpha / \gamma}} \frac{\|E_r w\|^2}{\Delta_r}. \tag{39}$$

Assume $\gamma = S_1 + \beta$ for some $\beta = o_n(S_1)$. Then, we require that

$$1 \ > \ \epsilon_1^{2-\alpha} + \frac{1}{1 + (\beta / S_1)} \underbrace{\left(\frac{1}{S_1} \sum_{r \geq 2} \frac{\|E_r w\|^2}{\Delta_r} \right)}_{=1} - \frac{1}{2\gamma} \sum_{\substack{r \geq 2: \\ \gamma < \epsilon_1^\alpha / \Delta_r}} \frac{\|E_r w\|^2}{\Delta_r}, \tag{40}$$

which is equivalent to

$$\frac{1}{2\gamma} \sum_{\substack{r \geq 2: \\ \gamma < \epsilon_1^\alpha / \Delta_r}} \frac{\|E_r w\|^2}{\Delta_r} + o_n(1) \ > \ \epsilon_1^{2-\alpha}. \tag{41}$$

Therefore, we may omit the $o_n(1)$ term as it suffices to satisfy

$$\frac{1}{2\gamma} \sum_{\substack{r \geq 2: \\ \gamma < \epsilon_1^\alpha / \Delta_r}} \frac{\|E_r w\|^2}{\Delta_r} \ > \ \epsilon_1^{2-\alpha} \quad \text{or} \quad \sum_{\substack{r \geq 2: \\ \gamma < \epsilon_1^\alpha / \Delta_r}} \frac{\|E_r w\|^2}{\epsilon_1^2} \frac{\epsilon_1^\alpha}{\gamma \Delta_r} \ > \ 2.$$

If $\epsilon_1 \leq c \|E_r w\|$, for all $r \geq 2$, the claim follows as $|I_\alpha| \geq 2c^2$. □

5.2 Near Perfect Fidelity

When the fidelity is $1 - o_n(1)$, we show that the principal perturbed eigenspace must have a significant overlap with the subspace spanned by the principal eigenspace and the target state.

Theorem 8 *Let (H, w, γ) be a tuplet. If H is γ-Groverian with fidelity $1 - o_n(1)$, then the principal eigenvector of $\gamma H + ww^\dagger$ is an equal superposition of w and the principal eigenvector of H, up to $o_n(1)$ terms.*

Proof. Let z_1 and y_1 be the principal eigenvectors of H and $\gamma H + ww^\dagger$, respectively. Thus, $E_1 = z_1 z_1^\dagger$ and $F_1 = y_1 y_1^\dagger$. Starting with Equation (33) and then applying Equation (27) with $p = 1$, we get

$$f(t) \;\leq\; 4\frac{\|F_1 w\|^4}{\delta_+^2}\,\|E_1 w\|^2 \;=\; 4\,\|E_1 F_1 w\|^2 \;=\; 4|\langle y_1, z_1\rangle|^2 |\langle y_1, w\rangle|^2.$$

If $f(t) = 1 - o_n(1)$, we obtain $1 - o_n(1) \leq 2|\langle y_1, z_1\rangle||\langle y_1, w\rangle|$. Since $|\langle y_1, z_1\rangle|^2 + |\langle y_1, w\rangle|^2 \leq 1 + o_n(1)$, we have $0 \leq (|\langle y_1, z_1\rangle| - |\langle y_1, w\rangle|)^2 = o_n(1)$, which proves the claim. □

6 Sufficient Gap

In this section, we prove our optimal characterization of S_1-Groverian graphs under a simpler assumption. First, we justify that the choice of $\gamma = S_1$ is almost best possible. By Equation (25) with $p = 1$, we have

$$1 = \frac{\epsilon_1^2}{\delta_+} + \sum_{r \neq 1} \frac{\|E_r w\|^2}{\delta_+ + \gamma\Delta_r} \asymp \epsilon_1 + \sum_{r \neq 1} \frac{\|E_r w\|^2}{\delta_+ + \gamma\Delta_r}$$

as $\epsilon_1 \asymp \delta_+$ is a necessary condition due to Theorem 5(i). Recall that $f_n \asymp g_n$ denotes that f_n and g_n are within constant factors of each other. Therefore,

$$1 - \epsilon_1 \asymp \frac{1}{\gamma}\sum_{r \neq 1} \frac{\|E_r w\|^2}{\Delta_r}\frac{1}{1 + (\epsilon_1/\gamma\Delta_r)}.$$

If $\gamma \gtrsim \sqrt{S_1}$, since $\epsilon_1 \ll \sqrt{S_1}\Delta_2$, we have $\epsilon_1/\gamma\Delta_r = o_n(1)$. This shows

$$\gamma(1 - \epsilon_1) \asymp \sum_{r \neq 1} \frac{\|E_r w\|^2}{\Delta_r}\frac{1}{1 + (\epsilon_1/\gamma\Delta_r)} = S_1(1 + o_n(1)).$$

As $\epsilon_1 = o_n(1)$, we have $\gamma \asymp S_1$.

The next theorem is our main characterization for optimal spatial search for $\gamma = S_1$.

Theorem 9 *Let (H, w, γ) be a tuplet where $\theta_2 \in \mathrm{Supp}_H(w)$. If $\epsilon_1 \ll \sqrt{S_1}\Delta_2$, then H is S_1-Groverian if and only if $S_2/S_1^2 \asymp 1$.*

Proof. By Lemma 2, we know that ζ_1 and ζ_2 are simple and $\zeta_1, \zeta_2 \notin \mathrm{Spec}(S_1 H)$. Therefore, let y_1 and y_2 be their corresponding eigenvectors. Define $\delta_+ = \zeta_1 - S_1$ and $\delta_- = \zeta_2 - S_1$. Also, let $\Delta_r = 1 - \theta_r$. Using Equation (25) with $p = 1, 2$, we derive

$$1 \;=\; \sum_{r=1}^{d} \frac{\|E_r w\|^2}{\zeta_p - S_1\theta_r} \;=\; \frac{\epsilon_1^2}{\delta_\pm} + \sum_{r=2}^{d} \frac{\|E_r w\|^2}{S_1\Delta_r}\frac{1}{1 + \delta_\pm/(S_1\Delta_r)}. \tag{42}$$

Note $(1+\alpha)^{-1} = 1 - \alpha + \alpha^2(1+\alpha)^{-1}$ holds for all $\alpha \neq -1$. Using $\alpha = \delta_\pm/(S_1\Delta_r)$, after reorganizing and cancelling terms, we arrive at

$$\frac{\epsilon_1^2}{\delta_\pm^2} \;=\; \frac{1}{S_1^2}\sum_{r=2}^{d}\frac{\|E_r w\|^2}{\Delta_r^2}\frac{S_1\Delta_r}{\delta_\pm + S_1\Delta_r}. \tag{43}$$

Thus far, this is similar to the first portion of the proof of Theorem 2 in [7]. But, now we exploit the sharper estimates given by Proposition 4 which will considerably simplify the rest of our proof.

Lemma 4 $\epsilon_1^2/\delta_\pm^2 \sim S_2/S_1^2$.

Proof. Proposition 4 shows that $|\delta_\pm| = O_n(\sqrt{S_1}\epsilon_1)$, and as $\epsilon_1 \ll \sqrt{S_1}\Delta_2$, we get $|\delta_\pm| \ll S_1\Delta_2$. Applying this to Equation (43) proves the claim. □

Lemma 5 $2\epsilon_1^2/\delta_+^2 \sim 1/\|F_1 w\|^2$ *and* $2\epsilon_1^2/\delta_-^2 \sim 1/\|F_2 w\|^2$.

Proof. We apply Equation (24) to ζ_1 and ζ_2, and after some rearrangements, we get

$$\frac{1}{\|F_p w\|^2} = \frac{\epsilon_1^2}{\delta_\pm^2} + \frac{1}{S_1^2}\sum_{r=2}^{d}\frac{\|E_r w\|^2}{\Delta_r^2}\frac{1}{(1+\delta_\pm/(S_1\Delta_r))^2} \qquad (p = 1,2). \tag{44}$$

Proposition 4 shows that $|\delta_\pm| = O_n(\sqrt{S_1}\epsilon_1)$, which combined with the assumption $\epsilon_1 \ll \sqrt{S_1}\Delta_2$ yields $|\delta_\pm| \ll S_1\Delta_2$. Applying this to Equation (44), we obtain

$$\frac{1}{\|F_p w\|^2} \;=\; \frac{\epsilon_1^2}{\delta_\pm^2} + \frac{S_2}{S_1^2}(1+o_n(1)) \;\sim\; \frac{2\epsilon_1^2}{\delta_\pm^2} \qquad (p=1,2), \tag{45}$$

as $\epsilon_1^2/\delta_\pm^2 \sim S_2/S_1^2$ by Lemma 4. □

The use of density matrices simplifies the proof of the following result as most arguments involving phase factors are no longer necessary.

Lemma 6 *If* $t = O_n(\sqrt{S_2}/S_1\epsilon_1)$, *then* $f(t) = \Omega_n(S_1/\sqrt{S_2})$.

Proof. By Equation (26), we have $E_1F_p w = \|F_p w\|^2 E_1 w/(\zeta_p - S_1)$. For $p = 1,2$, using Lemma 5 to replace $\|F_p w\|^2$, we obtain

$$\|E_1 F_p w\| = \|F_p w\|^2 \frac{\epsilon_1}{|\delta_\pm|} \sim \frac{|\delta_\pm|}{2\epsilon_1}. \tag{46}$$

Let $\delta = (\zeta_1 - \zeta_2)/2$. Then, the fidelity is given by

$$\begin{aligned} f(t) &= \mathrm{Tr}(ww^\dagger \sum_{p,q} e^{-it(\zeta_p - \zeta_q)} F_p E_1 F_q) \\ &= \sum_{p,q} e^{-it(\zeta_p-\zeta_q)} \langle E_1 F_p w, E_1 F_q w\rangle \\ &= \sum_{p,q} e^{-it(\zeta_p-\zeta_q)} \epsilon_1^2 \frac{\|F_p w\|^2}{\zeta_p - S_1} \frac{\|F_q w\|^2}{\zeta_q - S_1} \\ &= \frac{1}{2}(1-\cos(2\delta t))\frac{\delta^2}{\epsilon_1^2} + \epsilon_1^2 \sum_{p,q\neq 1,2} e^{-it(\zeta_p-\zeta_q)} \frac{\|F_p w\|^2}{S_1 - \zeta_p} \frac{\|F_q w\|^2}{S_1 - \zeta_q} \\ &\geq \frac{\delta^2}{\epsilon_1^2}, \quad \text{by setting } t = \tfrac{\pi}{2}\delta^{-1}. \end{aligned}$$

Now, note that $\delta = \frac{1}{2}(\delta_+ + |\delta_-|) \asymp \epsilon_1$. □

We have shown that if $S_1^2/S_2 = \Theta_n(1)$ then H is S_1-Groverian. It remains to show the converse.

Lemma 7 *If $f(t) = \Omega_n(1)$, for some $t = O_n(1/\epsilon_1)$, then $S_2/S_1^2 = \Theta_n(1)$.*

Proof. We prove the contrapositive. If $S_2/S_1^2 \not\asymp 1$, or equivalently, $\epsilon_1^2 \not\asymp \delta_+^2$ by Lemma 4, then H is not Groverian by Theorem 5(i). Note $\epsilon_1^2 \asymp \delta_+^2$ if and only if $\epsilon_1 \asymp \delta_+$. □

Lemma 6 and 7 completes the proof of the theorem. □

Remarks. We now compare Theorem 9 in the context of the known results in [6, 7]. Notice that Theorem 9 implies the main result (Lemma 1) in Chakraborty *et al.* [6]. Their result requires the constant gap condition $\Delta_2 = \Omega_n(1)$ which is a stronger assumption because of the following observation. In what follows, we denote $\epsilon_2 = \|E_2 w\|$.

Fact 10 *Suppose $\epsilon_1 = o_n(1)$. If $\Delta_2 = \Omega_n(1)$, then $S_1\Delta_2 = \Theta_n(1)$.*

Proof. Note $\epsilon_2^2 + \Delta_2(1 - \epsilon_1^2 - \epsilon_2^2) \leq S_1\Delta_2 \leq 1 - \epsilon_1^2$. The upper bound $S_1\Delta_2 = O_n(1)$ holds immediately. If $\epsilon_2 = o_n(1)$, then $S_1\Delta_2 = \Omega_n(1)$ follows as $\Delta_2 = \Omega_n(1)$. Otherwise, $S_1\Delta_2 = \Omega_n(1)$ holds from $\epsilon_2 = \Omega_n(1)$. □

We also note the following relation between S_1 and S_2 (which can be compared to Lemma 5 in [7]).

Fact 11 $S_1^2/S_2 \leq 1 - \epsilon_1^2$.

Proof. Consider a random variable Z where $Z = 1/\Delta_r$ with probability $\epsilon_r^2/(1-\epsilon_1^2)$, for $r = 2, \ldots, d$. Then, $\mathbb{E}[Z] = S_1/(1-\epsilon_1^2)$ and $\mathbb{E}[Z^2] = S_2/(1-\epsilon_1^2)$. Now, $\mathbb{E}[Z^2] \geq \mathbb{E}[Z]^2$ since variance is always nonnegative. □

Next, observe that $S_1 \geq 1 - \epsilon_1^2$. If $S_1 \leq 1$, then both S_1 and $\sqrt{S_1}$ are constant; otherwise, $\sqrt{S_1} \leq S_1$. To summarize, it is clear that $\sqrt{S_1} \lesssim S_1 \lesssim \sqrt{S_2}$.

As for the main result in Chakraborty *et al.* [7], their theorem requires the assumption $\epsilon_1 \ll S_1S_2/S_3$ and $\epsilon_1 \ll \sqrt{S_2}\Delta_2$. In Theorem 9, we replace these two assumptions with a single assumption $\epsilon_1 \ll \sqrt{S_1}\Delta_2$. The latter assumption is only slightly stronger than $\epsilon_1 \ll \sqrt{S_2}\Delta_2$ since under the regime of interest, namely, $S_2/S_1^2 = \Theta_n(1)$, they are asymptotically equivalent.

7 Examples

We analyze some examples of well-known families of graphs (see Figure 2). In order to simplify the calculations, we normalize the matrices as $H/\|H\|$ which places the eigenvalues in $[-1, 1]$ (instead of $[0, 1]$). Since the two normalizations are equal up to a factor of 2, this will not affect our asymptotic conclusions.

Graph Family	*Groverian?*	ϵ_1	Δ_2	S_1	*Comment*
Clique K_n	Yes	$n^{-1/2}$	1	1	$\Delta_2 = 1$
Expander	Yes	$n^{-1/2}$	1	-	$\Delta_2 = 1$
Strongly Regular Graph	Yes	$n^{-1/2}$	1	-	$\Delta_2 = 1$
Hamming $H(n, q)$	Yes	$q^{-n/2}$	$1/n$	1	$\epsilon_1 \ll \sqrt{S_1}\Delta_2$
Johnson $J(n, k)$	Yes	$n^{-k/2}$	$1/k$	1	$\Delta_2 = 1$
Grassmann $G_q(n, k)$	Yes	$q^{-k(n-k)/2}$	$1 - 1/q$	-	$\Delta_2 = 1$
Distance Regular Graph with classical parameters (d, q, α, β)	Yes	$1/\sqrt{\lvert V(G)\rvert}$	$1 - 1/q + \alpha/q\beta$	-	$\Delta_2 = 1$
Cycle C_n	No	$n^{-1/2}$	n^{-2}	n	$\epsilon_1 \not\ll \sqrt{S_1}\Delta_2$

Fig. 2. Examples of graph families and S_1-Groverian (or optimal spatial search) properties. Assume q, k, d are constants and $\alpha \ll \beta$. The expressions involving ϵ_1, Δ_2, and S_1 are asymptotic in nature. Some entries are missing as they do not impact the property.

Cliques The normalized eigenvalues of K_n are 1 (with multiplicity 1) and $-1/(n-1)$ (with multiplicity $n-1$). So, cliques are Groverian (in fact, with fidelity 1) since Δ_2 is constant. This was, of course, the original observation of Farhi and Gutmann [4].

Expanders A graph $G = (V, E)$ is called an (n, d, c)-expander if G has n vertices, maximum degree d, and for each set of vertices W of size $|W| \leq n/2$, we have $|N(W)| \geq c|W|$, where $N(W)$ is the set of vertices not in W but is adjacent to some vertex in W. Here, c is called the expansion which is required to be constant. It is known that if G is d-regular on n vertices, then it is a $(n, d, \Delta_2/2)$-expander provided $\Delta_2 = \Theta_n(1)$ (see [15]). So, expanders are Groverian since Δ_2 is constant. This is the main observation of Chakraborty *et al.* [6].

Strongly Regular Graphs A graph G_n is called *strongly regular* with parameter (n, k, a, c) if it is a k-regular on n vertices where every pair of adjacent vertices have a common neighbors and every pair of non-adjacent vertices have c common neighbors. Let $\theta_1 > \theta_2$ be the non-principal eigenvalues. Then, $k - c = \theta_1(-\theta_2)$, which implies $\theta_1 = (k - c)/(-\theta_2)$. If G_n is primitive but not a conference graph, then $-\theta_2 \geq 2$. Therefore, $\theta_1 \leq (k - c)/2 < k/2$. This shows that Δ_2 is constant. On the other hand, if G_n is a conference graph then $k = (n-1)/2$ and $\theta_1 = (\sqrt{n}-1)/2$ which implies $\Delta_2 = 1 - o_n(1)$. Thus, strongly regular graphs are Groverian. This provides an alternative proof of the result due to Janmark *et al.* [8].

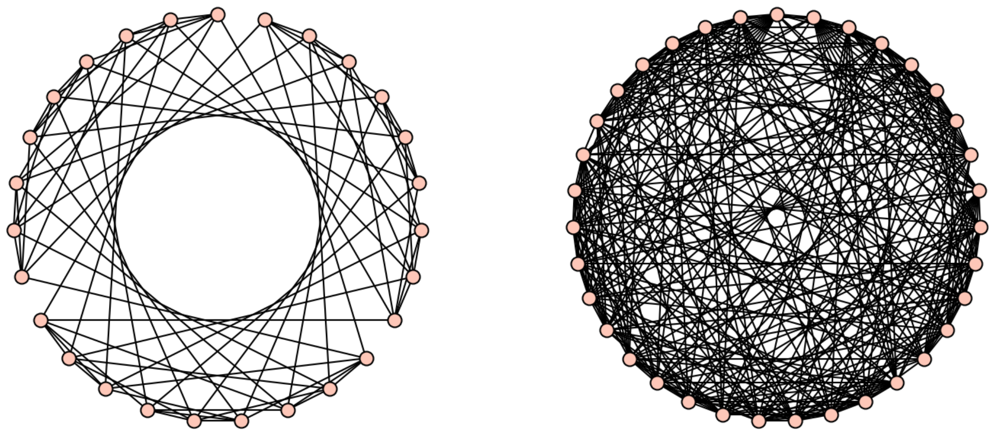

Fig. 3. Some distance-regular graphs that are Groverian: Hamming graphs $H(n,q)$ and Grassmann graphs $G_q(n,k)$, where q and k are constants. Left: Hamming graph $H(3,3)$. Right: Grassmann graph $G_2(4,2)$.

Hamming graphs The Hamming graph $H(n,q)$, with q is constant, has $(\mathbb{Z}/q\mathbb{Z})^n$ as its vertices where two n-tuples are connected if they differ in exactly one dimension. As $H(n,q)$ has q^n vertices with eigenvalues $\theta_r = n(q-1) - qr$ with multiplicity $m_r = \binom{n}{r}(q-1)^r$, for $r = 0, \dots, n$, we have $\Delta_2 = q/n(q-1) \sim 1/n$ and $\epsilon_1 = 1/q^{n/2}$. Since $S_1 = \Theta_n(1)$, the Hamming graph $H(n,q)$ is Groverian as $\epsilon_1 \ll \sqrt{S_1}\Delta_2$. To see why $S_1 = \Theta_n(1)$, notice that

$$S_1 = \frac{1}{q^n}\sum_{r=0}^{n}\binom{n}{r}\frac{n(q-1)}{rq}(q-1)^r \sim \frac{1}{q^n}\sum_{r}\binom{n+1}{r+1}(q-1)^r \asymp 1.$$

For the n-cube or $H(n,2)$, this was observed by Childs and Goldstone [5].

Johnson graphs The Johnson graph $J(n,k)$ has as its vertices the set of k-subsets of $\{1,\dots,n\}$, denoted $\binom{[n]}{k}$, where two k-subsets A and B are connected if $|A \cap B| = k-1$. So, $J(n,k)$ has $\binom{n}{k}$ vertices with eigenvalues $\theta_r = (k-r)(n-k-r) - r$ with multiplicity $m_r = \binom{n}{r} - \binom{n}{r-1}$, for $r = 0,\dots,k$. Notice $\epsilon_1 = 1/\sqrt{\binom{n}{k}} \sim n^{-k/2}$ and

$$\Delta_2 = \frac{\theta_0 - \theta_1}{\theta_0 - \theta_k} = \frac{n}{k(n-k+1)} \sim \frac{1}{k}$$

which is constant if k is. As $\Delta_2 = \Omega_n(1)$, this shows that $J(n,k)$, for $k \geq 3$, is Groverian. This recovers the results of Wong [9] and Tanaka *et al.* [10].

Grassmann graphs The Grassmann graph $G_q(n,k)$ has as its vertices the set of k-subspaces of the vector space $\mathbb{F}_q^n$ where two k-subspaces A and B are connected if $\dim(A \cap B) = k-1$. We assume $n \geq 2k$. The number of vertices of $G_q(n,k)$ is

$$N = \begin{bmatrix} n \\ k \end{bmatrix}_q \sim q^{k(n-k)}.$$

The eigenvalues are given by

$$\theta_r = q^{r+1}\begin{bmatrix}k-r\\1\end{bmatrix}_q\begin{bmatrix}n-k-r\\1\end{bmatrix}_q - \begin{bmatrix}r\\1\end{bmatrix}_q \sim q^{n-r-1}$$

with multiplicity

$$m_r = \begin{bmatrix}n\\r\end{bmatrix}_q - \begin{bmatrix}n\\r-1\end{bmatrix}_q,$$

for $r = 0, \ldots, k$. Notice $\epsilon_1 = 1/\sqrt{N}$ and the normalized eigenvalue gap is

$$\Delta_2 = 1 - \frac{\theta_1}{\theta_0} \sim 1 - \frac{1}{q},$$

which is constant if q is. As $\Delta_2 = \Omega_n(1)$, this shows that $G_q(n,k)$, for $k \geq 2$, is Groverian. Note $k = 1$ recovers the cliques.

Distance-regular graphs with classical parameters The eigenvalues of distance-regular graphs with classical parameters (d, q, α, β) are given in Jurišić and Vidali [16] (see Lemma 2). In particular, $\theta_0 = [d]_q\beta$ and $\theta_1 = [d-1]_q(\beta - \alpha) - 1$, which implies

$$\Delta_2 = 1 - \frac{[d-1]_q(\beta-\alpha)-1}{[d]_q\beta} \sim 1 - \frac{1}{q} + \frac{1}{q}\frac{\alpha}{\beta}$$

is constant provided $\alpha \ll \beta$.

Cycles The results from Section 5 can be used to prove that cycles are not Groverian. The normalized eigenvalues of C_n are given by $\theta_r = \frac{1}{2}(1 + \cos(2\pi(r-1)/n))$, $r = 1, \ldots, n$. Using $\cos(x) \sim 1 - x^2/2$, we have $\Delta_r \sim r^2/n^2$, for small positive values of r. Since C_n is a circulant, $\epsilon_r \sim 1/\sqrt{n}$ for all $r = 1, \ldots, n$. Note that

$$S_1 = \frac{1}{n}\sum_{r=1}^{n-1}\frac{1}{1-\cos(2\pi r/n)} \sim 2\int_{2\pi/n}^{\pi-2\pi/n}\frac{dx}{1-\cos(x)} = 2\cot(\pi/n) = \Theta_n(n).$$

Next, we show spatial search fails as γ ranges over all values.

Case (i). $\gamma = S_1 + \omega_n(\sqrt{n})$: Notice Theorem 6 applies since $\sqrt{n} = \epsilon_1 S_1 \ll \gamma - S_1 = \omega_n(\sqrt{n})$.

Case (ii). $\gamma = S_1 \pm o_n(n)$: Here, Theorem 7 applies since $\epsilon_1^\alpha/\Delta_r > S_1 + \beta$ holds, for $\alpha \in (1,2)$. With $|\beta| = o_n(n)$, evidently $n^{-\alpha/2} \times n^2 \gg cn \pm o_n(n)$.

Case (iii). $\gamma = O_n(n)$: To apply Theorem 7, we rewrite Equation (39) as

$$\frac{1}{2}\sum_{\substack{r\geq 2:\\ \Delta_r < \epsilon_1^\alpha/\gamma}}\frac{\epsilon_r^2}{\Delta_r} > \gamma\epsilon_1^{2-\alpha} + S_1 - \gamma, \tag{47}$$

since $\gamma > 0$. Because $\gamma = O_n(n)$, $S_1 = O_n(n)$, and $\epsilon_1 = 1/\sqrt{n}$, the right-hand side is at most $O_n(n)$. Next, we determine the set of indices r so that $\Delta_r < \epsilon_1^\alpha/\gamma$ which are included in the summation. The smallest the upper bound ϵ_1^α/γ can be is $1/n^{1+\alpha/2}$. We have

$$\Delta_r \sim \frac{r^2}{n^2} \ll \frac{1}{n^{1+\alpha/2}}, \quad \text{for } r = O_n(1).$$

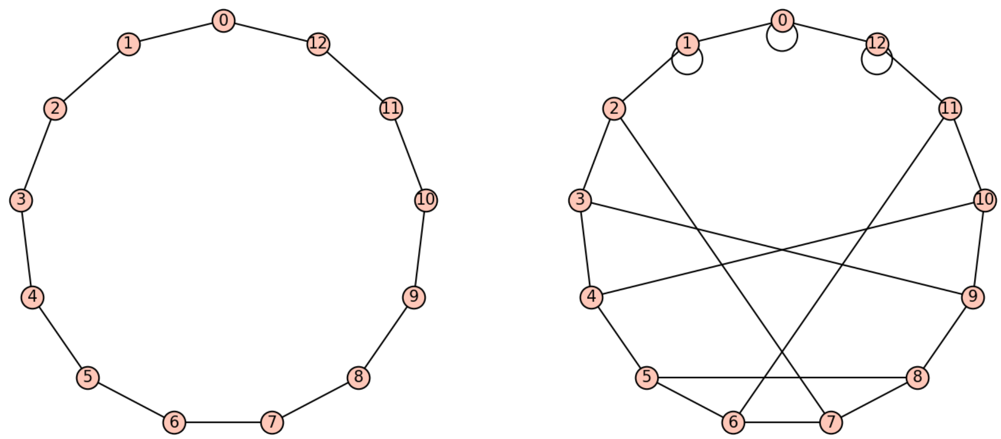

Fig. 4. Sparsity is not a good indicator: for prime p, C_p is not Groverian, but C_p with the extra "matching" $x \mapsto x^{-1} \pmod p$ is Groverian (as it is an expander, see Vadhan [17]). Left: C_{13}. Right: the nonsimple 3-regular expander C_{13} plus the modular inverse matching.

Thus, if we restrict the indices for which $r \le B$, for a large enough constant B, we get

$$\sum_{\substack{r\geq 2:\\ \Delta_r < \epsilon_1^{\alpha}/\gamma}} \frac{\epsilon_r^2}{\Delta_r} \;\geq\; \sum_{r=2}^{B} \frac{\epsilon_r^2}{\Delta_r} \;\sim\; \sum_{r=2}^{B} \frac{n^{-1}}{r^2 n^{-2}} \;=\; \Omega_n(n).$$

Thus, Equation (47) is satisfied provided B is large enough; whence spatial search fails.

8 Concluding remarks

In this work, we proved a simpler characterization of graphs with the optimal spatial search property (therein called Groverian). This improves a previous characterization obtained by Chakraborty *et al.* [7]. We applied this characterization to recover known results about some families of Groverian graphs and also to find new families of Groverian graphs. Along the way, we also proved a lower bound for spatial search on arbitrary graphs for constant fidelity. This extends a known lower bound due to Farhi and Gutmann [4] which holds for vertex transitive graphs and for fidelity that is one. We also developed a family of necessary conditions for a graph to be Groverian. Our necessary conditions, which are built upon observations developed by Chakraborty *et al.* [7], can be applied to provide rigorous proofs to show why some families of graphs (for example, cycles) lack the spatial search property.

We conclude with some open questions from the present work:

1. Is the Groverian property determined by spectra? Moreover, is the condition $\epsilon_1 \ll \sqrt{S_1}\Delta_2$ necessary for optimal characterization?

2. Can a family of graphs be Groverian with non-constant S_1? To the best of our knowledge, all families of graphs known to be Groverian satisfy $S_1 = \Theta_n(1)$.

3. When is the Groverian property (almost) periodic?

4. How robust is the Groverian property against noise? Regev and Schiff [18] had ruled this out for the discrete-time case.

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