

An Exponential Separation Between Quantum and Quantum-Inspired Classical Algorithms for Linear Systems

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Abstract

Achieving a provable exponential quantum speedup for an important machine learning task has been a central research goal since the seminal HHL quantum algorithm for solving linear systems and the subsequent quantum recommender systems algorithm by Kerenidis and Prakash. These algorithms were initially believed to be strong candidates for exponential speedups, but a lower bound ruling out similar classical improvements remained absent. In breakthrough work by Tang, it was demonstrated that this lack of progress in classical lower bounds was for good reasons. Concretely, she gave a classical counterpart of the quantum recommender systems algorithm, reducing the quantum advantage to a mere polynomial. Her approach is quite general and was named *quantum-inspired classical* algorithms. Since then, almost all the initially exponential quantum machine learning speedups have been reduced to polynomial via new quantum-inspired classical algorithms. From the current state-of-affairs, it is unclear whether we can hope for exponential quantum speedups for any natural machine learning task.

In this work, we present the first such provable exponential separation between quantum and quantum-inspired classical algorithms for the basic problem of solving a linear system when the input matrix is well-conditioned and has sparse rows and columns.

1 Introduction

Demonstrating an exponential quantum advantage for a relevant machine learning task has been an important research goal since the promising quantum algorithm by Harrow, Hassidim and Lloyd [15] for solving linear systems. Ignoring a few details, the HHL algorithm (and later improvements [4, 10]) generates a quantum state $\sum_{i=1}^n x_i|i\rangle$ corresponding to the solution $x = M^{-1}y$ to an $n \times n$ linear system of equations $Mx = y$ in just $\text{poly}(\ln n)$ time. At first sight, this seems exponentially faster than any classic algorithm, which probably has to read the entire input matrix M to solve the same problem. However, as pointed out e.g. by Aaronson [1], the analysis of the HHL algorithm assumes the input matrix is given in a carefully chosen input format. Taking this *state preparation* into consideration, it was initially unclear how the performance could be compared to a classical algorithm and whether any quantum advantage remained.

The shortcoming of the HHL algorithm regarding state preparation was later addressed in several works, with one of the first and most thorough treatments in the thesis of Prakash [24]. Prakash introduced a framework where input matrices and vectors to a linear algebraic machine learning problem are given as simple classical data structures, but with quantum access to the memory representations. This allows for a direct comparison to classical data structures where the input is given in the same data structure. Expanding on these ideas, Kerenidis and Prakash [17] presented a quantum recommender systems algorithm that was exponentially faster than the best classical counterpart. Their algorithm was one of the strongest candidates for a provable exponential quantum advantage and sparked a fruitful line of research, yielding exponential speedups for a host of important machine learning tasks, including solving linear systems [7], linear regression [7], PCA [7], recommender systems [17], supervised clustering [18] and Hamiltonian simulation [14].

Despite the exponential speedups over classical algorithms, a lower bound for classical algorithms ruling out a similar improvement via new algorithmic ideas remained elusive. It turned out that this was for good

reasons: In breakthrough work by Tang [27], it was demonstrated that on all inputs where the recommender systems algorithm by Kerenidis and Prakash yielded an exponential speedup, a similar speedup could be obtained via a classical algorithmic approach that she dubbed *quantum-inspired classical* (QIC) algorithms. Since then, almost all the initially exponential speedups from quantum algorithms have been reduced to mere polynomial speedups through the development of new efficient QIC algorithms, see e.g. [6, 8, 25]. The disheartening state-of-affairs is thus that only a few machine learning problems remain where there is still an exponential gap between quantum and QIC algorithms. Based on Tang’s work, it remains entirely plausible that new QIC algorithms may close these gaps as well.

Our Contribution. In this work, we present the first provable exponential separation between quantum and quantum-inspired classical algorithms for the central problem of solving linear systems with sparse rows and columns. The lower bound is exponentially higher than known quantum upper bounds [11] when the matrix is well-conditioned, thus establishing the separation.

1.1 Quantum-Inspired Classical Algorithms

In the following, we formally introduce QIC algorithms, the linear system problem, our lower bound statement and previous work on proving separations between quantum and QIC algorithms.

As mentioned earlier, the work by Prakash [24], and later work by Kerenidis and Prakash [17], gave rigorous frameworks for directly comparing a quantum algorithm for a machine learning task with a classical counterpart. Taking state preparation into account, Kerenidis and Prakash define a natural input format (data structure) for matrices and vectors in linear algebraic problems. At a high level, they assume the input is presented as a classical binary tree based data structure over the entries of the rows and columns of a matrix. They then built their quantum recommender system algorithm assuming quantum access to the memory representation of this classical data structure. Follow-up works have used essentially the same input representation or equivalent formulations. In many cases, for sufficiently well-conditioned matrices, the obtained quantum algorithms run in just $\text{poly}(\ln n)$ time.

Now to prove a separation between quantum and classical algorithms, any fair comparison should use the same input representation. Given the simplicity of the data structure by Kerenidis and Prakash for representing the input, it seemed reasonable to conjecture that any classical algorithm for e.g. recommender systems would need polynomial time even when given this data structure. This intuition was however proven false by Tang [27]. Her key insight was that the classical data structure allows efficient classical (i.e. $\text{poly}(\ln n)$ time) ℓ_2 sampling (formally defined below) from the rows and columns of the input, as well as efficient reading of individual entries. Exploiting this sampling access, she gave a classical algorithm for recommender systems that runs in just $\text{poly}(\ln n)$ time on all matrices where the quantum algorithm by Kerenidis and Prakash does. She referred to such classical algorithms with ℓ_2 sampling access to input matrices and vectors as *quantum-inspired classical* algorithms. This sampling access has since then proved extremely useful in other machine learning tasks, see e.g. [6, 8, 25]. Tang [27] summarized the above discussion as follows: “*when quantum machine learning algorithms are compared to classical machine learning algorithms in the context of finding speedups, any state preparation assumptions in the quantum machine learning model should be matched with ℓ_2 -norm sampling assumptions in the classical machine learning model*”.

Using the notation of Mande and Shao [21], QIC algorithms formally have the following access to the input:

Definition 1 (Query Access). *For a vector $v \in \mathbb{R}^n$, we have $Q(v)$, query access to v , if for all i , we can query v_i . Likewise for a matrix $M \in \mathbb{R}^{m \times n}$, we have query access to M if for all $(i, j) \in [m] \times [n]$, we can query $M_{i,j}$.*

Definition 2 (Sampling and Query Access to a Vector). *For a vector $v \in \mathbb{R}^n$, we have $SQ(v)$, sampling and query access to v , if we can*

- *Query for entries of v as in $Q(v)$.*

- Obtain independent samples of indices $i \in [n]$, each distributed as $\mathbb{P}[i] = v_i^2 / \|v\|^2$.
- Query for $\|v\|$.

Definition 3 (Sampling and Query Access to a Matrix). For a matrix $M \in \mathbb{R}^{m \times n}$, we have $SQ(M)$ if we have $SQ(M_{i,\star})$, $SQ(M_{\star,j})$, $SQ(r)$ and $SQ(c)$ for all $i \in m$ and $j \in n$ where $r(M) = (\|M_{1,\star}\|, \dots, \|M_{m,\star}\|)$ and $c(M) = (\|M_{\star,1}\|, \dots, \|M_{\star,n}\|)$. Here $M_{i,\star}$ is the i 'th row of M , $M_{\star,j}$ is the j 'th column, $r(M)$ is the vector of row-norms and $c(M)$ is the vector of column-norms of M .

In the above definitions, and throughout the paper, we use $\|x\|$ to denote the ℓ_2 norm $\|x\|_2$. With the input representation defined, we proceed to present the problem of solving a linear system via a QIC algorithm. Here one again needs to be careful for a fair comparison between quantum and QIC algorithms. Concretely, the known quantum algorithms for solving a linear system $Mx = y$ do not output the full solution x (which would take linear time), but instead a quantum state $\sum_i \tilde{x}_i |i\rangle$ for a \tilde{x} approximating the solution x . Taking measurements on such a state allows one to sample an index i with probability $\tilde{x}_i^2 / \|\tilde{x}\|^2$. With this in mind, the classical analog of solving a linear system is as follows.

Problem 1 (Linear Systems). Given $SQ(M)$ and $SQ(y)$ for a symmetric and real matrix $M \in \mathbb{R}^{n \times n}$ of full rank, a vector $y \in \mathbb{R}^n$ and precision $\varepsilon > 0$, the Linear Systems problem is to support sampling an index i with probability $\tilde{x}_i^2 / \|\tilde{x}\|^2$ from a vector \tilde{x} satisfying that $\|\tilde{x} - x\| \leq \varepsilon \|x\|$ where $x = M^{-1}y$ is the solution to the linear system of equations $Mx = y$.

The query complexity of a QIC algorithm for solving a linear system, is the number of queries to $SQ(M)$ and $SQ(y)$ necessary to sample one index i from \tilde{x} . We remark that the known QIC algorithms furthermore output the value \tilde{x}_i upon sampling i . Since we aim to prove a lower bound, our results are only stronger if we prove it for merely sampling i .

Quantum Benchmark. To prove our exponential separation, we first present the state-of-the-art performance of quantum algorithms for linear systems. Here we focus on the case where the input matrix M has sparse rows and columns, i.e. every row and column has at most s non-zero entries. The running time of the best known quantum algorithm depends on the condition number of M , defined as

$$\kappa = \sigma_{\max} / \sigma_{\min}.$$

Here σ_{\max} is the largest singular value of M and σ_{\min} is the smallest singular value. Note that for real symmetric M of full rank, all eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$ of M are real and non-zero, and the singular values $\sigma_{\max} = \sigma_1 \geq \dots \geq \sigma_n = \sigma_{\min} > 0$ are the absolute values of the eigenvalues $\{|\lambda_i|\}_{i=1}^n$ in sorted order. Given a precision $\varepsilon > 0$, matrix M and vector y as input (in the classical data structure format), the quantum algorithm by Costa et al. [11] (improving over previous works, e.g. [7]) runs in time

$$O(\kappa \ln(1/\varepsilon) \min\{s, \sqrt{s}(\kappa s/\varepsilon)^{o(1)}\}) \quad (1)$$

to produce a quantum state $\sum_i \tilde{x}_i |i\rangle$ for a \tilde{x} with $\|\tilde{x} - x\| \leq \varepsilon \|x\|$ with $x = M^{-1}y$. We remark that to derive (1) from [7], one invokes either a reduction from [14] (for the s guarantee) or [20] (for the $\sqrt{s}(\kappa s/\varepsilon)^{o(1)}$ guarantee) to obtain a block-encoding of a sparse matrix. See also the recent work [19] for high success probability guarantees.

QIC Benchmark. For QIC algorithms, the best bound is due to [25] and has a query complexity (and running time) of

$$\text{poly}(s, \kappa_F, \ln(1/\varepsilon), \ln n), \quad (2)$$

where

$$\kappa_F = \|M\|_F / \sigma_{\min} = \frac{\sqrt{\sum_i \sigma_i^2}}{\sigma_{\min}}.$$

Since κ_F may be larger than κ by as much as a \sqrt{n} factor, there are thus matrices with $\kappa, s = \text{poly}(\ln n)$ where there is an exponential gap between (1) and (2).

An alternative upper bound for a closely related problem was given by Gharibian and Le Gall [13] and is based on the quantum singular value decomposition. In more detail, they show that for a matrix M where $M^\dagger M$ has eigenvalues $1 = \lambda_1 \geq \dots \geq \lambda_n = \kappa^{-1}$, if we apply a degree d polynomial P to the square-roots of the eigenvalues (and maintain the same eigenvectors) to obtain a matrix $P(\sqrt{M^\dagger M})$ with eigenvalues $P(\lambda_1^{1/2}), \dots, P(\lambda_n^{1/2})$, then given sampling and query access to M and two vectors u and v of unit norm, it is possible to classically estimate the number $u^\dagger P(\sqrt{M^\dagger M})v$ to within additive ϵ in roughly $O(s^{2d}/\epsilon^2)$ time. Since x^{-1} can be well-approximated in the interval $[-1, 1] \setminus [-\kappa^{-1}, \kappa^{-1}]$ by a degree $d = O(\kappa \log(\kappa/\epsilon))$ polynomial, this essentially allows us to estimate $u^\dagger M^{-1}v$. This is not quite sampling from $M^{-1}v$ but reasonably close. Furthermore, it suggests that to achieve an exponential separation between QIC and quantum algorithms, we probably need to consider κ that is at least logarithmic in n . See the discussion below for a similar recent result by Montanaro and Shao and more details.

In light of the above, it is clear that for many settings of parameters κ, κ_F and ϵ , there is still an exponential gap between the quantum and QIC upper bounds. However it has still not been proved unconditionally that such a gap is inherent.

Our Result. We show the following strong lower bound for QIC algorithms

Theorem 1. *There is a constant $c > 0$, such that for $n \geq c$ and any precision $\epsilon \leq (c\sqrt{\ln n})^{-1}$, it holds that for any QIC algorithm \mathcal{A} for linear systems, there exists a full rank $n \times n$ symmetric real matrix M with condition number $\kappa \leq c \ln n$ and 3-sparse rows and columns, such that \mathcal{A} must make $\Omega(n^{1/4}/\ln^{3/2} n)$ queries to $SQ(M)$ on the linear system $Mx = e_1$.*

Observe that the complexity of the best quantum algorithm (1) for this setting of s, κ and ϵ is just $\ln(n) \ln \ln n$, hence the claimed exponential separation. Furthermore, the matrix M is extremely sparse, with only $s = 3$ non-zeros per row and column, and the vector y in the linear system $Mx = y$ is simply the first standard unit vector e_1 .

Let us also remark that our lower bound also holds in the well-studied *sparse access model*, see e.g. [14, 12]. In the sparse access model, we can query for the i 'th non-zero of any row or column of M and all rows and columns have at most s non-zeros.

Previous Hardness of Solving Linear Systems. In the seminal HHL paper [15] that introduced the first quantum algorithm for solving linear systems, the authors also proved conditional lower bounds for classical algorithms. Concretely, they proved that solving a sparse and well-conditioned linear system is BQP-complete (bounded-error quantum polynomial time). For this result, the assumption is that the matrix is presented to the algorithm as a short binary encoding (a $\text{poly}(\ln n)$ bit encoding of an $n \times n$ matrix). Assuming the widely-believed conjecture that $\text{BQP} \neq \text{P}$, this implies that there is no polynomial time classical algorithm for the same problem and input representation. Since QIC access to the matrix can be efficiently simulated from such a binary encoding, this implies a *conditional* separation between quantum and QIC algorithms for linear systems. Our new lower bound is however *unconditional* and gives an explicit gap ($\ln(n) \ln \ln n$ vs. $n^{1/4}/\ln^{3/2} n$) in terms of the number of oracle queries without relying on computational hardness assumptions. However, it is reasonable to say that the HHL result hints that an unconditional separation was within reach.

Previous Lower Bounds for QIC Algorithms. Prior to our work, there has been several works proving lower bounds for QIC and related algorithms, although none of them establishing the exponential separation for linear systems that we give in this work. In the following, we review the most relevant such works.

Recent work by Mande and Shao [21] also study linear systems among several other problems. Using reductions from number-in-hand multiparty communication complexity [23], they prove a number of lower bounds for QIC algorithms for linear regression (and systems), supervised clustering, PCA, recommender systems and Hamiltonian simulation. Their lower bounds are of the form $\tilde{\Omega}(\kappa_F^2)$, but only for problems

where the best known quantum algorithms are no better than $\tilde{O}(\kappa_F)$, thus establishing quadratic separations compared to our exponential separation. Let us also remark that our lower bound proof takes a completely different approach, instead reducing from a problem of random walks by Childs et al. [9], or alternatively, from Simon's problem [26].

Andoni, Krauthgamer and Pongrow [5] also studied the problem of approximating the solution to a linear system in sub-linear time via sampling access to the non-zero entries of M and y . However, instead of requiring that the output index is sampled from a vector \tilde{x} with $\|x - \tilde{x}\| \leq \varepsilon\|x\|$, they make the stronger requirement that for any query index i , the algorithm must approximate x_i to within additive $\varepsilon\|x\|_\infty$. Note that this is both a harder problem in terms of the goal of approximating every single entry of x , and the error guarantee in terms of $\varepsilon\|x\|_\infty$ is much stricter than our $\varepsilon\|x\|$. Proving lower bounds for their problem is thus seemingly an easier task. In particular, their hard instance is trivial to solve with additive $\varepsilon\|x\|$ error for $\varepsilon = n^{-o(1)}$ as one can simply output 0 to approximate x_i for any i .

Very recently, Montanaro and Shao [22] studied the sparse access model for the problem of estimating entries of $f(M)$. Here $f : [-1, 1] \rightarrow [-1, 1]$ is a function that can be approximated by a polynomial and $f(M)$ for a Hermitian M with $\|M\| \leq 1$ (all eigenvalues bounded by 1 in absolute value) with eigendecomposition UDU^\dagger , is the matrix $Uf(D)U^\dagger$ with f applied entrywise on the diagonal entries of D . In particular, for $f(x) = x^{-1}$, we have that $f(M)$ is the inverse M^{-1} . Montanaro and Shao show that the quantum query complexity of estimating entries of $f(M)$ is bounded by a polynomial in $\widehat{\deg}_\varepsilon(f)$, where $\widehat{\deg}_\varepsilon(f)$ is the least degree of a real-valued polynomial P such that $|P(x) - f(x)| \leq \varepsilon$ for all $x \in [-1, 1]$. On the other hand, they also prove that classical algorithms must query $\exp(\Omega(\widehat{\deg}_\varepsilon(f)))$ many entries. This result does not directly apply to the matrix inverse problem since $f(x) = x^{-1}$ is not bounded by 1 in absolute value for $x \in [-1, 1]$. Montanaro and Shao discuss this shortcoming and observe that if all eigenvalues of M are at least κ^{-1} in absolute value (corresponding to condition number κ), then $f(x) = x^{-1}$ can be approximated in $[-1, 1] \setminus [-\kappa^{-1}, \kappa^{-1}]$ by a polynomial of degree $O(\kappa \log(\kappa/\varepsilon))$. However, this is an upper bound, not a lower bound on the approximate degree, and they mention that they are not aware of any lower bound on the approximate degree of $f(x) = x^{-1}$ when restricted to $[-1, 1] \setminus [-\kappa^{-1}, \kappa^{-1}]$. An appropriate rescaling of M together with this upper bound result thus hints that the condition number κ must be at least logarithmic in the matrix size to establish an exponential separation for estimating entries of M^{-1} to within additive ε . On the other hand, for general f with approximate degree at least logarithmic, their results give exponential separations between classical and quantum algorithms for estimating entries of $f(M)$ in the sparse access model.

2 Separation

We prove our lower bound result in Theorem 1 via a reduction from either a problem by Childs et al. [9] on random walks in graphs, or from the classic Simon's problem [26]. While the reduction from Simon's problem gives the tightest lower bound, we believe both reductions have value. In particular, we find that the reduction from random walks is simpler and more self-contained. Furthermore, the proof via random walks provides novel new insights into the graph construction by Childs et al. [9]. We hope these insights may find further applications and have therefore chosen to include both reductions. We start by presenting our reduction from random walks.

Childs et al. [9] study the following oracle query problem. There is an unknown input graph. The graph is obtained by constructing two perfect binary trees T_1 and T_2 of height n each, i.e. they have 2^n leaves. The leaves of the two trees are connected by a uniformly at random chosen alternating cycle. That is, if we fix an arbitrary leaf ℓ_1 in tree T_1 , then the cycle is obtained by connecting ℓ_1 to a uniform random leaf in T_2 , that leaf is then again connected to a uniform random remaining leaf in T_1 and so forth, always alternating between the two trees. When no more leaves remain and we are at leaf ℓ_2 in T_2 , the cycle is completed by adding the edge back to ℓ_1 .

The $N = 2^{n+2} - 2$ nodes of T_1 and T_2 are now assigned uniform random and distinct $2n$ bit labels, except the root of T_1 that is assigned the all-0 label. Call the resulting random graph G_n .

Childs et al. now consider the following game: We are given query access to an oracle \mathcal{O} . Upon receiving a $2n$ -bit query string x , \mathcal{O} either returns that no node of the two trees has the label x , or if such a node exists, the labels of its neighbors are returned. The game is won if \mathcal{O} is queried with the label of the root of T_2 . Otherwise it is lost. Throughout the paper, we use i^* to denote the (random) $2n$ -bit label of the root of T_2 . Childs et al. [9] prove the following lower bound for any classical algorithm that accesses the graph G_n only through the oracle \mathcal{O} :

Theorem 2 (Childs et al. [9]). *Any classical algorithm that queries \mathcal{O} at most $2^{n/6}$ times wins with probability at most $4 \cdot 2^{-n/6}$.*

The key idea in our lower bound proof is to use an efficient QIC algorithm for linear systems to obtain an efficient classical algorithm for the above random walk game. As a technical remark, Childs et al. also included a random *color* on each edge of G_n and this color was also returned by \mathcal{O} . The colors were exploited in a quantum upper bound making only $\text{poly}(n)$ queries to the oracle to win the game with good probability. Since providing an algorithm with less information only makes the problem harder, the lower bound in Theorem 2 clearly holds for our variant without colors as well.

2.1 Reduction from Random Walks

Assume we have a QIC algorithm \mathcal{A} for linear systems that makes $T(M, \varepsilon)$ queries to $SQ(M)$ to sample an index from \tilde{x} such that each index i is sampled with probability $\tilde{x}_i^2 / \|\tilde{x}\|^2$ for a \tilde{x} satisfying $\|\tilde{x} - x\| \leq \varepsilon \|x\|$ for a sufficiently small $\varepsilon > 0$. Here $x = M^{-1}y$ is the solution to the equation $Mx = y$. Our idea is to carefully choose a matrix M (and vector y) depending on the random graph G_n represented by \mathcal{O} , such that simulating all calls of \mathcal{A} to $SQ(M)$ and $SQ(y)$ via calls to the oracle \mathcal{O} , \mathcal{A} will output a sample index i that with sufficiently large probability equals the index i^* of the root of T_2 . Said differently, the coordinate \tilde{x}_{i^*} of \tilde{x} corresponding to the root i^* of T_2 is sufficiently large. Making a final query to \mathcal{O} with i then wins the game with good probability.

Let us first describe the simulation and the matrix M . We consider the $2^{2n} \times 2^{2n}$ matrix M whose rows and columns correspond to the possible $2n$ -bit labels in the graph G_n . Let B be the $N \times N$ submatrix of M corresponding to the (random) labels of the $N = 2^{n+2} - 2$ actual nodes in G_n . If A denotes the adjacency matrix of the graph G_n (nodes ordered as in B), then we let $B = \lambda I - A$ for a parameter λ to be determined. For all rows/columns of M not corresponding to nodes in G_n , we let the diagonal entry be $\sqrt{\lambda^2 + 3}$ and all off-diagonals be 0. Note that we are not explicitly computing the matrix M to begin with. Instead, we merely argue that by querying \mathcal{O} , we can simulate \mathcal{A} as if given access to $SQ(M)$.

Clearly M is symmetric and real and thus has real eigenvalues and eigenvectors. Furthermore, we will choose λ such that M has full rank (which is if and only if all its eigenvalues are non-zero). Also observe that every row/column not corresponding to the two roots of T_1 and T_2 , has norm $\sqrt{\lambda^2 + 3}$ (every node of T_1 and T_2 , except the roots, have degree 3).

Our goal is now to use the QIC algorithm \mathcal{A} for linear systems with $SQ(M)$ and $SQ(e_{0\dots 0})$ as input, to give an algorithm for the oracle query game with oracle \mathcal{O} for G_n . Here $e_{0\dots 0}$ is the standard unit vector corresponding to the root node of T_1 which always has the all-0 label. For short, we will assume this is the first row/column of M and write $e_1 = e_{0\dots 0}$.

Simulating $SQ(M)$. We now argue how to simulate each of the queries on $SQ(M)$ and $SQ(e_1)$ made by \mathcal{A} via calls to \mathcal{O} . $SQ(e_1)$ is trivial to implement as e_1 is known and requires no calls to \mathcal{O} .

For $SQ(M)$, to sample an index from a row $M_{i,*}$ or column $M_{*,j}$, we query \mathcal{O} for all nodes adjacent to i (or j). If \mathcal{O} returns that i is not a valid label, we return the entry i (corresponding to sampling the only non-zero entry of $M_{i,*}$, namely the diagonal). Otherwise, \mathcal{O} returns the list of neighbors of i . We know that row i (column j) has λ in the diagonal and -1 in all entries corresponding to neighbors. We can thus sample from $M_{i,*}$ with the correct distribution and pass the result to \mathcal{A} . To query an entry $M_{i,j}$ of M , we simply query \mathcal{O} for the node i . If \mathcal{O} returns that i is not a valid label, we return $\sqrt{\lambda^2 + 3}$ if $j = i$ and otherwise return 0. If \mathcal{O} returns the neighbors of i , then if $j = i$, we return λ , if j is among the neighbors, we return -1 and otherwise we return 0.

We support sampling from $r(M)$ and $c(M)$ by returning a uniform random index among the 2^{2n} rows/columns. This requires no queries to \mathcal{O} . Note that this *almost* samples from the correct distribution: Every node v of G_n that is not a root of the two trees, is adjacent to three nodes. Hence the norm of the corresponding row and column is precisely $\sqrt{\lambda^2 + 3}$. This is the same norm as all rows and columns of M not corresponding to G_n (i.e. rows and columns outside the submatrix B). Hence the distribution of a sample from $r(M)$ and $c(M)$ is uniform random if we condition on not sampling an index corresponding to a root. Conditioned on never sampling a root in our simulation, the simulation of all samples from $r(M)$ and $c(M)$ follow the same distribution as if we used the correct sampling probabilities for $r(M)$ and $c(M)$. The probability we sample one of the two roots is at most $2T(M, \varepsilon)2^{-2n}$ and we subtract this from the success probability of the simulation.

Finally, when the simulation of \mathcal{A} terminates with an output index i , we query \mathcal{O} for i (with the hope that i equals the index i^* of the root of T_2). We thus have

Observation 1. *Given a precision $\varepsilon > 0$ and a QIC algorithm \mathcal{A} for linear systems making $T(M, \varepsilon)$ queries to $SQ(M)$, there is a classical algorithm for random walks in two binary trees that makes at most $T(M, \varepsilon) + 1$ queries to the oracle \mathcal{O} , where M is the matrix defined from G_n . Furthermore, it wins the game with probability at least $\tilde{x}_{i^*}^2 / \|\tilde{x}\|^2 - 2T(M, \varepsilon)2^{-2n}$ for a \tilde{x} satisfying $\|\tilde{x} - x\| \leq \varepsilon\|x\|$ with $x = M^{-1}e_1$ the solution to the linear system $Mx = e_1$ and i^* the index of the root of T_2 .*

What remains is thus to determine an appropriate λ , to argue that M has a small condition number, to find a suitable $\varepsilon > 0$ and to show that $\tilde{x}_{i^*}^2 / \|\tilde{x}\|^2$ is large. This is done via the following two auxiliary results

Lemma 1. *The adjacency matrix A of the graph G_n has no eigenvalues in the range $(\sqrt{8}, 3 - 2^{-n}]$.*

Lemma 2. *If λ is chosen as $\sqrt{8} + \gamma$ for a $0 < \gamma \leq \left(\frac{1}{16(n+2)}\right)^2$ and $n \geq c$ for a sufficiently large constant $c > 0$, then $x_{i^*}^2 = \Omega(n^{-5}\|x\|^2)$ where $x = M^{-1}e_1$ is the solution to the linear system $Mx = e_1$ and i^* is the index of the root of T_2 .*

Before proving these results and motivating the bounds they claim, we use them to complete our reduction and derive our lower bound. In light of Lemma 2, we choose $\lambda = \sqrt{8} + \gamma$ with $\gamma = 1/(16(n+2))^2$. Let us now analyse the condition number of M . First, note that the sum of absolute values in any row or column of M is no more than $\max\{\sqrt{\lambda^2 + 3}, \lambda + 3\} \leq 6$. Thus the largest singular value of M is at most 6. For the smallest singular value, observe that M is block-diagonal with B in one block and $\sqrt{\lambda^2 + 3} \cdot I$ in the other. The latter has all singular values $\sqrt{\lambda^2 + 3} > 3$. For B , we first observe that any row and column of the adjacency matrix A has sum of absolute values at most 3. Hence the eigenvalues of A lie in the range $[-3, 3]$. From Lemma 1, we now have that all eigenvalues of $B = \lambda I - A$ lie in the ranges $[\lambda - 3, \lambda - 3 + 2^{-n}] \subseteq [-0.18, -0.17]$ (for n sufficiently large) and $(\lambda - \sqrt{8}, \lambda + 3] \subseteq (\gamma, 6)$. We thus have that the smallest singular value (smallest absolute value of an eigenvalue) of M is at least $\gamma = 1/(16(n+2))^2$. The condition number κ is thus at most $6 \cdot (16(n+2))^2$ (recall that the size of the matrix is 2^{2n} , thus the condition number is only polylogarithmic in the matrix size).

Let us next analyse \tilde{x} . From Lemma 2 we have that $|\tilde{x}_{i^*}| \geq |x_{i^*}| - \varepsilon\|x\| = |x_{i^*}| - O(\varepsilon n^{2.5}|x_{i^*}|)$. For $\varepsilon \leq (cn^{2.5})^{-1}$ for sufficiently large constant c , this is at least $|x_{i^*}|/2 = \Omega(n^{-2.5}\|x\|)$ by Lemma 2. Furthermore, by the triangle inequality, we have $\|\tilde{x}\| \leq (1 + \varepsilon)\|x\|$, and hence $\tilde{x}_{i^*}^2 / \|\tilde{x}\|^2 = \Omega(n^{-5})$. We thus win the random walk game with probability at least

$$\Omega(n^{-5}) - 2T(M, \varepsilon)2^{-2n}.$$

For n sufficiently large, this implies that either $T(M, \varepsilon) \geq 2^{n/6}$ or this success probability is greater than $4 \cdot 2^{-n/6}$. Thus Theorem 2 by Childs et al. [9] and Observation 1 gives us that the number of queries, $T(M, \varepsilon) + 1$, must be at least $2^{n/6}$. This establishes Theorem 1 with slightly worse parameters as the size of M is $2^{2n} \times 2^{2n}$ (i.e. with $\kappa \leq c \ln^2 n$, $\varepsilon \leq (c \ln^{2.5} n)^{-1}$, 4-sparse rows and columns and $\Omega(n^{1/12})$ queries on an $n \times n$ matrix). Our later reduction from Simon's problem (in Section 3), improves these parameters by polynomial factors.

Motivating the Construction. Before we proceed to give proofs in Section 4, let us make a number of comments on the intuition behind our concrete choice of matrix M and the bounds claimed in Lemma 1 and Lemma 2. In light of the reduction from the random walk problem, it is clear that we should choose a matrix M such that we can 1.) simulate $SQ(M)$ via \mathcal{O} , 2.) guarantee a small condition number of M , and 3.) guarantee that $\tilde{x}_{i^*}^2/\|\tilde{x}\|^2$ is as large as possible.

Condition 1. naturally hints at using the adjacency matrix A of G_n as part of the construction of M since querying \mathcal{O} precisely retrieves the neighbors and thus non-zero entries of a row or column of A . It further guarantees sparse rows and columns in M . For condition 2., we have to introduce something in addition to A as the eigenvalues of A lie in the range $[-3, 3]$, but we have no guarantee that they are sufficiently bounded away from 0. A natural choice is $B = \lambda I - A$ as this shifts the eigenvalues to lie in the range $[\lambda - 3, \lambda + 3]$. Setting the entries of M outside the submatrix corresponding to the actual nodes in G_n to $\sqrt{\lambda^2 + 3}$ is again a natural choice as this makes sampling from $c(M)$ and $r(M)$ trivial. From this alone, it would seem that $\lambda \gg 3$ would be a good choice. Unfortunately, such a choice of λ would not guarantee condition 3. To get an intuition for why this is the case, recall that \tilde{x} is ε -close to $x = M^{-1}e_1$. Since M is block-diagonal, with B the block containing the first row and $\sqrt{\lambda^2 + 3} \cdot I$ the other block, x is non-zero only on coordinates corresponding to the block B . Abusing notation, we thus write $x = B^{-1}e_1$. Thus what we are really interested in showing, is that $x_{i^*}^2/\|x\|^2$ is large for this x . Examining the linear system $Bx = e_1$, we see that all rows corresponding to internal nodes v of T_1 and T_2 define an equality. The equality states that the entry x_v corresponding to v must satisfy $\lambda x_v - x_{p(v)} - x_{\ell(v)} - x_{r(v)} = 0$ where $p(v)$ is the parent of v , $\ell(v)$ the left child and $r(v)$ the right child (for leaves of T_1 and T_2 , the children are the neighboring leaves in the opposite tree). Since this pattern is symmetric across the nodes of T_1 and T_2 , it is not surprising that x is such that all nodes v on the j 'th level of T_i have the same value $x_v = \psi_j^{(i)}$. Let us focus on the tree T_2 and simplify the notation by dropping the index and letting $\psi_j \leftarrow \psi_j^{(2)}$. From the above, the ψ_j 's satisfy the constraints $\lambda\psi_{j+1} - \psi_j - 2\psi_{j+2} = 0$. A recurrence $a\psi_{j+2} + b\psi_{j+1} + c\psi_j = 0$ is known as a *second degree linear recurrence* and when $b^2 > 4ac$ its solutions are of the form

$$\psi_j = \alpha \cdot \left(\frac{-b + \sqrt{b^2 - 4ac}}{2a} \right)^j + \beta \cdot \left(\frac{-b - \sqrt{b^2 - 4ac}}{2a} \right)^j,$$

where $\alpha, \beta \in \mathbb{R}$ are such that ψ_1 and ψ_2 satisfy any initial conditions one might require. For our construction, we have $a = -2, b = \lambda$ and $c = -1$, resulting in

$$\psi_j = \alpha \cdot \left(\frac{\lambda - \sqrt{\lambda^2 - 8}}{4} \right)^j + \beta \cdot \left(\frac{\lambda + \sqrt{\lambda^2 - 8}}{4} \right)^j.$$

Since the root of T_2 does not have a parent, the corresponding equality from $Mx = e_1$ gives the initial condition $\lambda\psi_1 - 2\psi_2 = 0$, implying $\psi_1 = (2/\lambda)\psi_2$. If we work out the details, this can be shown to imply $\alpha = -\beta$ in any solution to the recurrence and thus

$$\psi_j = \alpha \cdot \left(\left(\frac{\lambda - \sqrt{\lambda^2 - 8}}{4} \right)^j - \left(\frac{\lambda + \sqrt{\lambda^2 - 8}}{4} \right)^j \right).$$

For λ sufficiently larger than $\sqrt{8}$, the term $((\lambda + \sqrt{\lambda^2 - 8})/4)^j$ is at least a constant factor larger in absolute value than $((\lambda - \sqrt{\lambda^2 - 8})/4)^j$ and we have

$$\psi_j \approx -\alpha \cdot \left(\frac{\lambda + \sqrt{\lambda^2 - 8}}{4} \right)^j. \quad (3)$$

For $\lambda \geq 3$, we therefore roughly have that $|\psi_j| \geq |\psi_{j-1}| \cdot (3 + \sqrt{9 - 8})/4 = |\psi_{j-1}|$. But there are 2^j nodes of depth j in T_2 , thus implying that the magnitude of $x_{i^*}^2$, with i^* the root of T_2 , is no more than $\|x\|^2 2^{-n}$.

This is far too small for both the sampling probability $x_{i^*}^2/\|x\|^2$ and the required precision ε such that simply setting $\tilde{x}_{i^*} \leftarrow 0$ in \tilde{x} does not violate $\|\tilde{x} - x\| \leq \varepsilon\|x\|$.

To remedy this, consider again (3) and let us understand for which values of λ that $x_{i^*}^2$ is not significantly smaller than $\|x\|^2$. If we could choose $\lambda = \sqrt{8}$ (technically we require $b^2 > 4ac$ and thus $\lambda > \sqrt{8}$), then (3) instead gives $|\psi_j| \approx |\psi_{j-1}| \cdot \sqrt{8}/4$ and thus $\|x\|^2 \approx \sum_{j=0}^{n-1} 2^j (\sqrt{8}/4)^{2j} x_{i^*}^2 = nx_{i^*}^2$. This is much better as the size of the matrix M is 2^{2n} and thus an ε that is only inverse polylogarithmic in the matrix size suffices to sample i^* with large enough probability to violate the lower bound for the random walk game. Notice also that choosing $\lambda = \sqrt{8} + c$ for any constant $c > 0$ is insufficient to cancel the exponential growth in number of nodes of depth j (as for $\lambda \geq 3$). Thus we are forced to choose λ very close to $\sqrt{8}$.

Unfortunately choosing $\lambda \approx \sqrt{8}$ poses other problems. Concretely the eigenvalues of B then lie in the range $[\sqrt{8} - 3, \sqrt{8} + 3]$, which contains 0 and thus we are back at having no guarantee on the condition number. However even if A has eigenvalues in the range $[-3, 3]$, it is not given that there are eigenvalues spread over the entire range. In particular, since all nodes of G_n , except the roots, have the same degree 3, we can almost think of G_n as a 3-regular graph. For d -regular graphs, the best we can hope for is that the graph is Ramanujan, i.e. all the eigenvalues of the adjacency matrix A , except the largest, are bounded by $2\sqrt{d-1}$ in absolute value (the second largest eigenvalue for any d -regular graph is at least $2\sqrt{d-1} - o(1)$, see [2]). For $d = 3$, this is precisely $\sqrt{8}$. In our case, the graph G_n is sadly *not* Ramanujan, as in addition to the largest eigenvalue of roughly 3 (only roughly since our graph is not exactly 3-regular), it also has an eigenvalue of roughly -3 . However, in Lemma 1 we basically show that this is the *only* other eigenvalue that does not lie in the range $[-\sqrt{8}, \sqrt{8}]$.

In light of the above, we wish to choose λ as close to $\sqrt{8}$ as possible, but not quite $\lambda = \sqrt{8}$ as we may then again risk having an eigenvalue arbitrarily close to 0. If we instead choose $\lambda = \sqrt{8} + \gamma$ for a small $\gamma > 0$, then (3) gives us something along the lines of

$$|\psi_j| \approx |\psi_{j-1}| \cdot \left(\frac{\sqrt{8} + \sqrt{8 + 2\sqrt{8}\gamma + \gamma^2 - 8}}{4} \right) = |\psi_{j-1}| \cdot \frac{\sqrt{8}}{4} \cdot (1 + O(\sqrt{\gamma})),$$

and thus $\|x\|^2 \approx \sum_{j=0}^{n-1} 2^j (\sqrt{8}/4)^{2j} (1 + O(\sqrt{\gamma}))^{2j} x_{i^*}^2 = nx_{i^*}^2 \exp(O(n\sqrt{\gamma}))$. Choosing $\gamma = O(1/n^2)$ as suggested in Lemma 2 thus recovers the desirable guarantee $\|x\|^2 = O(x_{i^*}^2 n)$ while yielding a condition number of no more than $O(n^2)$. Since the size of the matrix is $2^{2n} \times 2^{2n}$, this is only polylogarithmic in the matrix size. This completes the intuition behind our choice of parameters and results.

What remains is thus to formalize the above intuition and prove Lemma 1 and Lemma 2. This is postponed to Section 4, and in the next section, we instead give the alternative reduction from Simon's problem.

3 Reduction from Simon's

Here we give an alternative reduction, starting from the famous Simon's problem [26] and using the ideas in the proof by Harrow, Hassidim and Lloyd [15] that solving linear systems is BQP-complete. We start by recalling the main ideas in the two works.

HHL's BQP-Hardness Reduction. In [15], the authors consider a general reduction for simulating any quantum circuit via solving a linear system. We will outline their approach here using their notation. Assume we have a quantum circuit acting on n qubits. Let U_1, \dots, U_T denote the sequence of $2^n \times 2^n$ unitaries corresponding to the sequence of one- or two-qubit gates applied by the circuit on the initial state $|0\rangle^{\otimes n}$. They now consider the matrix

$$U = \sum_{t=1}^T |t\rangle\langle t-1| \otimes U_t + |t+T\rangle\langle t+T-1| \otimes I + |t+2T \bmod 3T\rangle\langle t+2T-1| \otimes U_{T+1-t}^\dagger.$$

For intuition on this construction, think of the matrix as being partitioned into a $3T \times 3T$ grid of sub-matrices of size $2^n \times 2^n$ each and notice how $|i\rangle\langle j| \otimes A$ places the matrix A as the sub-matrix in position (i, j) (with 0-indexed rows and columns $i, j \in [3T]$). A $3T \cdot 2^n$ -dimensional vector is similarly partitioned into $3T$ blocks. For $1 \leq t \leq T$, observe that the vector $U^t|0\rangle|0\rangle^{\otimes n}$ has the state of the n qubits after the first t steps of computation stored in its $t+1$ 'st block, and all other blocks are 0. Note that the first $|0\rangle$ in $|0\rangle|0\rangle^{\otimes n}$ refers to the $3T$ -dimensional standard unit vector with a 1 in its first entry. For $T \leq t \leq 2T-1$, $U^t|0\rangle|0\rangle^{\otimes n}$ simply has the final state of the qubits in the $t+1$ 'st block. Finally, for $2T \leq t \leq 3T-1$, the $t+1$ 'st block is undoing the computations until finally wrapping back around and recovering the initial state $|0\rangle|0\rangle^{\otimes n}$.

Harrow, Hassidim and Lloyd now consider the following matrix $A = I - Ue^{-1/T}$ and observe that its condition number is $O(T)$ and its inverse is given by

$$A^{-1} = \sum_{k=0}^{\infty} U^k e^{-k/T}. \quad (4)$$

Hence if we consider the solution to the linear system $Ax = |0\rangle|0\rangle^{\otimes n}$, then it is given by

$$x = A^{-1}|0\rangle|0\rangle^{\otimes n} = \sum_{k=0}^{\infty} U^k e^{-k/T} |0\rangle|0\rangle^{\otimes n} = \sum_{t=0}^{3T-1} U^t |0\rangle|0\rangle^{\otimes n} \sum_{k=0}^{\infty} e^{-(t+3Tk)/T}.$$

The crucial observation is now that the terms $U^t|0\rangle|0\rangle^{\otimes n}$ for $t = T, \dots, 2T-1$ has the final state of the computation in its $t+1$ 'st block and 0 elsewhere. Furthermore, since the U^t 's are unitaries and the $U^t|0\rangle|0\rangle^{\otimes n}$ are disjoint in their non-zeros, it follows that if we sample and index i from x with probability $x_i^2/\|x\|^2$, then the sample is from one of the blocks $T+1, \dots, 2T$ with probability

$$\frac{\sum_{t=T}^{2T-1} \left(\sum_{k=0}^{\infty} e^{-(t+3Tk)/T} \right)^2}{\sum_{t=1}^{3T-1} \left(\sum_{k=0}^{\infty} e^{-(t+3Tk)/T} \right)^2} = \Omega(1). \quad (5)$$

When this happens, the remaining n bits in the index i is a sample from the output state of the circuit. To finally obtain a symmetric matrix M , they define it as

$$M = \begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix} \quad (6)$$

and remark that its inverse is

$$M^{-1} = \begin{pmatrix} 0 & (A^{-1})^\dagger \\ A^{-1} & 0 \end{pmatrix}. \quad (7)$$

Simon's Problem. We now want to use the above reduction in combination with on an oracle query problem to prove our lower bound for QIC algorithms. For this, consider Simon's problem in which we have an oracle function $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ with the promise that either f is one-to-one, or it is two-to-one with $f(a) = f(b)$ if and only if $a = b \oplus s$ for a common $s \in \{0, 1\}^n$. Here \oplus denotes bitwise XOR. The goal is to determine whether f is one-to-one or two-to-one. This problem is known to require $\Omega(2^{n/2})$ classical oracle queries for success probability at least $1/2$.

Now recall the Simon's quantum algorithm for solving this problem. Represent the oracle f by a $2^{2n} \times 2^{2n}$ unitary U_f with rows and columns indexed by pairs (a, b) of two n -bit strings. Column (a, b) has a 1 in position $(a, b \oplus f(a))$ and 0 elsewhere. Note that this also implies that row (a, b) has a one in column $(a, b \oplus f(a))$ and 0 elsewhere. Simon's algorithm now operates on $2n$ qubits, starting in the initial state $|0\rangle^{\otimes n}|0\rangle^{\otimes n}$. It first applies n one-qubit Hadamard gates on the first n qubits to bring the state to

$$(H^{\otimes n} \otimes I^{\otimes n})|0\rangle^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{2^{n/2}} \sum_{j=0}^{2^n-1} |j\rangle|0\rangle^{\otimes n}.$$

It then applies the oracle U_f to bring the state to

$$U_f(H^{\otimes n} \otimes I^{\otimes n})|0\rangle^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{2^{n/2}} \sum_{j=0}^{2^n-1} |j\rangle |f(j)\rangle.$$

Finally, it applies n one-qubit Hadamard gates on the first n qubits again, to give the final state

$$\begin{aligned} (H^{\otimes n} \otimes I^{\otimes n})U_f(H^{\otimes n} \otimes I^{\otimes n})|0\rangle^{\otimes n}|0\rangle^{\otimes n} &= \frac{1}{2^{n/2}} \sum_{j=0}^{2^n-1} (H^{\otimes n}|j\rangle) |f(j)\rangle \\ &= \frac{1}{2^{n/2}} \sum_{j=0}^{2^n-1} \left(\frac{1}{2^{n/2}} \sum_{k=0}^{2^n-1} (-1)^{\langle j,k \rangle} |k\rangle \right) |f(j)\rangle \\ &= \sum_{j=0}^{2^n-1} |j\rangle \left(\frac{1}{2^n} \sum_{k=0}^{2^n-1} (-1)^{\langle j,k \rangle} |f(k)\rangle \right). \end{aligned}$$

In the above, $\langle j, k \rangle$ denotes inner product of the n -bit representations of j and k . We notice that if f is one-to-one, then the vector corresponding to this final state has $\pm 2^{-n}$ in each of its 2^{2n} entries. If on the other hand it is two-to-one with $f(a) = f(b)$ for $a = b \oplus s$, then for each of the 2^{n-1} values z in the image of f , if $f(a) = f(b) = z$ then $(-1)^{\langle j,a \rangle} = (-1)^{\langle j,b \oplus s \rangle} = (-1)^{\langle j,b \rangle + \langle j,s \rangle}$. It follows that if $\langle j, s \rangle$ is even, then $(-1)^{\langle j,a \rangle} = (-1)^{\langle j,b \rangle}$ and otherwise $(-1)^{\langle j,a \rangle} = -(-1)^{\langle j,b \rangle}$. In summary, the vector $(H^{\otimes n} \otimes I^{\otimes n})U_f(H^{\otimes n} \otimes I^{\otimes n})|0\rangle^{\otimes n}|0\rangle^{\otimes n}$ is $\pm 2/2^n$ in each entry corresponding to a pair $|j\rangle|k\rangle$ with $\langle j, s \rangle \equiv 0 \pmod 2$ and k in the image of f , and it is 0 elsewhere.

Combining HHL and Simon's. We now let U_1, \dots, U_n in the HHL reduction be the unitaries corresponding to the application of the first n one-qubit Hadamard gates in Simon's algorithm. Then we let $U_{n+1} = U_f$ and finally let U_{n+2}, \dots, U_{2n+1} be the application of the last n one-qubit Hadamard gates. We thus have $T = 2n + 1$ and may define the matrices A and M from (6). The matrix M is an $N \times N$ real symmetric matrix with $N = 2 \cdot 3T \cdot 2^{2n}$ and condition number $O(n) = O(\ln N)$.

Similarly to the reduction we gave in Section 2.1, assume we have a QIC algorithm \mathcal{A} that makes $T(M, \varepsilon)$ queries to $SQ(M)$ to sample an index from \tilde{x} such that each index i is sampled with probability $\tilde{x}_i^2 / \|\tilde{x}\|^2$ for a \tilde{x} satisfying $\|\tilde{x} - x\| \leq \varepsilon \|x\|$ for a sufficiently small $\varepsilon > 0$. Here $x = M^{-1}e_1$ is the solution to the linear system $Mx = e_1$. By the structure of M^{-1} from (7) and A^{-1} from (4), we see that

$$x = M^{-1}e_1 = \begin{pmatrix} 0 \\ A^{-1}|0\rangle|0\rangle^{\otimes 2n} \end{pmatrix}.$$

We will now simulate the QIC algorithm by making classical oracle queries to the function f . For this, we first observe that every row and every column of U has unit length and all its diagonal entries are 0. This further implies that the rows and columns of $A = I - Ue^{-1/T}$ and M all have the same norm. Thus if the QIC algorithm \mathcal{A} samples a row or column, we can simply return a uniform random index of a row or column. Next, if \mathcal{A} samples an index in a row or column proportional to the square of the index, we have two cases. If the row or column does not correspond to the oracle matrix U_f , then we can directly determine the entries of the row or column and simulate the sample without any oracle queries to f . Finally, if the row or column corresponds to a row or column (a, b) of U_f , we query the oracle for $f(a)$ and thereby determine the non-zero corresponding to $(a, b \oplus f(a))$. We can again correctly simulate a sample from the row/column. Thus the number of classical queries to f is at most $T(M, \varepsilon)$ to draw one sample from \tilde{x} .

Recall now that we can think of the vector $y = A^{-1}|0\rangle|0\rangle^{\otimes 2n}$ as consisting of $3T$ blocks y^t with $y = \sum_{t=0}^{3T-1} |t\rangle \otimes y^t$ and each y^t a 2^{2n} -dimensional vector. Furthermore, y^T, \dots, y^{2T-1} all equal the final state of Simon's algorithm. If we now use \mathcal{A} to draw an index $i = |t\rangle|j\rangle|k\rangle$ from \tilde{x} (with $t \in [3T], j \in [2^n], k \in [2^n]$), we first check if $t \in \{T, \dots, 2T-1\}$. Assume for now that $\tilde{x} = x$. Then we know from (5) that this

happens with $\Omega(1)$ probability. If this is the case, we know that (j, k) is uniformly random among pairs with $\langle j, s \rangle \equiv 0 \pmod 2$ and k in the image of f . If f is one-to-one, this is still the case, but with s the all-zero vector $\mathbf{0}$.

As in Simon's original algorithm, we now repeat the above sampling for cn times for a constant $c > 0$. For $c > 0$ large enough, it holds with overwhelming probability that if $s = \mathbf{0}$, then we see n linearly independent vectors $j \in \mathbb{F}_2^n$. If $s \neq \mathbf{0}$, then we see at most $n - 1$ linearly independent vectors as all returned j are orthogonal to s . We can thus determine whether f is one-to-one or two-to-one and the algorithm makes $O(nT(M, \varepsilon))$ many classical queries to f .

Handling Approximation. In the above, we assumed samples were from the exact solution x . If instead \tilde{x} has $\|x - \tilde{x}\| \leq \varepsilon\|x\|$, we have that the total ℓ_2 mass of indices $i = |t\rangle|j\rangle|k\rangle$ with $t \in \{T, \dots, 2T - 1\}$ but $\langle j, s \rangle \equiv 1 \pmod 2$ is no more than $\varepsilon\|x\|$. Call such indices i *invalid*. Furthermore, for ε less than a sufficiently small constant, the total ℓ_2 mass of indices $i = |t\rangle|j\rangle|k\rangle$ with $i \in \{T, \dots, 2T - 1\}$ and $\langle j, s \rangle \equiv 0 \pmod 2$ is $\Omega(\|x\|)$. Thus for each sample from \tilde{x} , the chance we get an invalid i is no more than $O(\varepsilon^2)$. A union bound over all cn samples drawn implies that for $\varepsilon < n^{-1/2}/c$ for a big enough constant $c > 0$, we can correctly distinguish f being one-to-one from two-to-one with probability larger than $1/2$. Since the input matrix size is $N \times N$ with $N = O(n^2 2^{2n})$, this is $\varepsilon < (c \ln^{1/2}(N))^{-1}$. We thus conclude

$$nT(M, \varepsilon) = \Omega(2^{n/2}) \Rightarrow T(M, \varepsilon) = \Omega(N^{1/4} / \ln^{3/2} N).$$

This gives us our main result in Theorem 1.

4 Spectral Properties of Random Walk Matrix

In this section we use Lemma 1 and Lemma 2 needed for our reduction from the random walk problem by Childs et al.

4.1 Bounding the Eigenvalues of the Adjacency Matrix

We start by proving Lemma 1, i.e. that the adjacency matrix A of the graph G_n has no eigenvalues in the range $(\sqrt{8}, 3 - 2^{-n}]$.

Let us first introduce some terminology. We say that the root of T_1 is at level 1, the leaves of T_1 at level $n + 1$, the leaves of T_2 at level $n + 2$ and the root of T_2 is at level $2n + 2$. Note that this is unlike the definition of $\psi_j^{(i)}$ in the previous section, where we focused on a single tree T_i and counted the level from the root of T_i and down. From hereon, it is more convenient for us to think of the level as the distance from the root of T_1 (with the root at level 1). The two roots have degree two and all other nodes have degree three.

To bound the eigenvalues of A , we begin with an observation that allows us to restrict our attention to so-called *layered* eigenvectors (inspired by previous works bounding eigenvalues of trees [16, 3]). We say that an eigenvector w is a layered eigenvector, if all entries of w corresponding to nodes at level i have the same value ϕ_i . We argue that

Observation 2. *If A has an eigenvector of eigenvalue λ , then it has a real-valued layered eigenvector of eigenvalue λ .*

Proof. Let u be an arbitrary eigenvector with eigenvalue λ . Since A is real and symmetric, its eigenvalues are real. If u is complex, we may write it as $u = v + ia$ with v and a real vectors. Since $Av + iAa = Au = \lambda u = \lambda v + i\lambda a$, it must be the case that $Av = \lambda v$ as these are the only real vectors in $Av + iAa$ and $\lambda v + i\lambda a$. By the same argument, we also have $Aa = \lambda a$. Thus v and a are real eigenvectors with eigenvalue λ . Assume wlog. that v is non-zero.

We now show how to construct a real layered eigenvector w from v having the same eigenvalue λ . First recall that a vector v is an eigenvector of A with eigenvalue λ , if and only if $(\lambda I - A)v = 0$. Now given the eigenvector v , let S_i be the set of coordinates corresponding to nodes in level i and let $\phi_i = w_j =$

$|S_i|^{-1} \sum_{k \in S_i} v_k$ for all $j \in S_i$. We will verify that $(\lambda I - A)w = 0$, which implies that w is also an eigenvector of eigenvalue λ .

For this, consider a level i and define $p_i \in \{0, 1, 2\}$ as the number of neighbors a node in level i has in level $i - 1$. Similarly, define $c_i \in \{0, 1, 2\}$ as the number of neighbors a node in level i has in level $i + 1$. To verify that $(\lambda I - A)w = 0$, we verify that for all levels i , we have $\lambda\phi_i - p_i\phi_{i-1} - c_i\phi_{i+1} = 0$. To see this, observe that since $(\lambda I - A)v = 0$, it holds for every index $j \in S_i$ that $\lambda v_j - \sum_{k \in S_{i-1}: j \in \mathcal{N}(k)} v_k - \sum_{k \in S_{i+1}: j \in \mathcal{N}(k)} v_k = 0$, where $\mathcal{N}(k)$ denotes the neighbors of k . Summing this across all nodes $j \in S_i$, we see that $\lambda \sum_{k \in S_i} v_k - c_{i-1} \sum_{k \in S_{i-1}} v_k - p_{i+1} \sum_{k \in S_{i+1}} v_k = 0$. This follows since every node k in level $i - 1$ has v_k included precisely c_{i-1} times in the sum (p_{i+1} times for nodes in level $i + 1$).

The left hand side also equals $\lambda\phi_i|S_i| - c_{i-1}\phi_{i-1}|S_{i-1}| - p_{i+1}\phi_{i+1}|S_{i+1}|$ by definition of ϕ_i . Now observe that $c_{i-1}|S_{i-1}| = p_i|S_i|$ since both sides of the equality equals the number of edges between levels $i - 1$ and i . Using this, we rewrite $0 = \lambda\phi_i|S_i| - c_{i-1}\phi_{i-1}|S_{i-1}| - p_{i+1}\phi_{i+1}|S_{i+1}| = \lambda\phi_i|S_i| - p_i\phi_{i-1}|S_i| - c_i\phi_{i+1}|S_i| = |S_i|(\lambda\phi_i - p_i\phi_{i-1} - c_i\phi_{i+1})|S_i|$. Since $|S_i| \neq 0$, we conclude $\lambda\phi_i - p_i\phi_{i-1} - c_i\phi_{i+1} = 0$. \square

Using Observation 2 it thus suffices for us to argue that A has no real-valued layered eigenvectors with eigenvalues in the range $(\sqrt{8}, 3 - 2^{-n}]$. The first step in this argument, is to lower bound the largest eigenvalue λ_1 . For this, recall that $\lambda_1 = \max_{v: \|v\|=1} v^T A v$. Noting that A is $N \times N$ with $N = 2^{n+2} - 2$, we now consider the unit vector v with all entries $1/\sqrt{N}$. Then $(Av)_i = 3/\sqrt{N}$ for i not one of the two roots, and $(Av)_i = 2/\sqrt{N}$ for i one of the two roots. Hence

$$\lambda_1 \geq 3 - 2/N > 3 - 2^{-n}. \quad (8)$$

Next, we aim to understand the structure of all real-valued layered eigenvectors of eigenvalues larger than $\sqrt{8}$. So let w be an arbitrary such eigenvector of eigenvalue $\lambda > \sqrt{8}$ and let ϕ_i denote the value of the coordinates of w corresponding to level i . Our goal is to show that $\lambda > \sqrt{8}$ implies $\lambda > 3 - 2^{-n}$.

Since $(\lambda I - A)w = 0$, we conclude from the row of A corresponding to the root of T_1 that $\lambda\phi_1 - 2\phi_2 = 0 \Rightarrow \phi_2 = (\lambda/2)\phi_1$. For levels $1 \leq i \leq n$, we must have $\lambda\phi_{i+1} - \phi_i - 2\phi_{i+2} = 0$. As discussed earlier, a recurrence $a\phi_{i+2} + b\phi_{i+1} + c\phi_i = 0$ is known as a second degree linear recurrence and when $b^2 > 4ac$ its (real) solutions are of the form

$$\phi_i = \alpha \cdot \left(\frac{-b + \sqrt{b^2 - 4ac}}{2a} \right)^i + \beta \cdot \left(\frac{-b - \sqrt{b^2 - 4ac}}{2a} \right)^i,$$

with $\alpha, \beta \in \mathbb{R}$ such that the initial condition $\phi_2 = (\lambda/2)\phi_1$ is satisfied. Note that in our case, $a = -2, b = \lambda$ and $c = -1$. Since we assume $\lambda > \sqrt{8}$, we indeed have $b^2 > 4ac$. It follows that

$$\phi_i = \alpha \cdot \left(\frac{\lambda - \sqrt{\lambda^2 - 8}}{4} \right)^i + \beta \cdot \left(\frac{\lambda + \sqrt{\lambda^2 - 8}}{4} \right)^i,$$

for α, β satisfying $\phi_2 = (\lambda/2)\phi_1$. For short, let us define $\Delta = \sqrt{\lambda^2 - 8}$. Note that Δ is real since we assume $\lambda > \sqrt{8}$. Furthermore, we have $\lambda - \Delta > 0$ and thus in later equations, it is safe to divide by $\lambda - \Delta$.

The initial condition now implies that we must have

$$\begin{aligned} \alpha \cdot \left(\frac{\lambda - \Delta}{4} \right)^2 + \beta \cdot \left(\frac{\lambda + \Delta}{4} \right)^2 &= (\lambda/2) \left(\alpha \cdot \frac{\lambda - \Delta}{4} + \beta \cdot \frac{\lambda + \Delta}{4} \right) \Rightarrow \\ \alpha \cdot (\lambda - \Delta)^2 + \beta \cdot (\lambda + \Delta)^2 &= 2\lambda (\alpha \cdot (\lambda - \Delta) + \beta \cdot (\lambda + \Delta)) \Rightarrow \\ \beta \cdot (\lambda^2 + \Delta^2 + 2\lambda\Delta - 2\lambda(\lambda + \Delta)) &= \alpha \cdot (-\lambda^2 - \Delta^2 + 2\lambda\Delta + 2\lambda(\lambda - \Delta)) \Rightarrow \\ \beta \cdot (-\lambda^2 + \Delta^2) &= \alpha \cdot (\lambda^2 - \Delta^2) \Rightarrow \\ \beta &= -\alpha. \end{aligned}$$

Thus the solutions have the following form for any $\alpha \in \mathbb{R}$:

$$\begin{aligned}\phi_i &= \alpha \cdot \left(\left(\frac{\lambda - \Delta}{4} \right)^i - \left(\frac{\lambda + \Delta}{4} \right)^i \right) \\ &= \alpha \left(\frac{\lambda - \Delta}{4} \right)^i \cdot \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^i \right)\end{aligned}\tag{9}$$

for $1 \leq i \leq n + 2$.

Now observe that the same equations apply starting from the root of T_2 and down towards the leaves of T_2 (recall our convention that the root of T_2 is at level $2n + 2$), thus for $1 \leq i \leq n + 2$

$$\phi_{2n+3-i} = \alpha' \left(\frac{\lambda - \Delta}{4} \right)^i \cdot \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^i \right).\tag{10}$$

Examining (9) and (10), we first notice that

$$\left(\frac{\lambda - \Delta}{4} \right)^i \cdot \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^i \right) < 0.\tag{11}$$

Furthermore, both (9) and (10) give bounds on the leaf levels ϕ_{n+1} and ϕ_{n+2} and these must be equal. Any non-zero solution thus must have $\alpha \cdot \alpha' > 0$, i.e. the two have the same sign. From (9), (10) and (11) it now follows that all pairs ϕ_i and ϕ_j satisfy $\phi_i \cdot \phi_j > 0$.

Now let v_1 be a layered and real-valued eigenvector corresponding to the largest eigenvalue λ_1 (such a layered eigenvector is guaranteed to exist by Observation 2). Let ψ_i denote the values of the entries in v_1 corresponding to nodes of level i . Since $\lambda_1 > \sqrt{8}$, the values ψ_i satisfy $\psi_i \cdot \psi_j > 0$ for all pairs ψ_i and ψ_j by the above arguments. Since eigenvectors corresponding to distinct eigenvalues of real symmetric matrices are orthogonal, we must have that either $\lambda = \lambda_1$ or $v_1^T w = 0$. But

$$\begin{aligned}(v_1^T w)^2 &= \left(\sum_{i=1}^{2n+2} 2^{\min\{i-1, 2n+2-i\}} \phi_i \psi_i \right)^2 \\ &= \sum_{i=1}^{2n+2} \sum_{j=1}^{2n+2} 2^{\min\{i-1, 2n+2-i\}} 2^{\min\{j-1, 2n+2-j\}} \phi_i \phi_j \psi_i \psi_j \\ &> 0.\end{aligned}$$

We thus conclude $\lambda = \lambda_1 > 3 - 2^{-n}$.

4.2 Understanding the Solution

In this section, we prove Lemma 2. That is, we show that for $\lambda = \sqrt{8} + \gamma$ with $0 < \gamma \leq \left(\frac{1}{16(n+2)} \right)^2$, it holds that $x_{i^*}^2 = \Omega(n^{-5} \|x\|^2)$ where $x = M^{-1}e_1$ is the solution to the linear system $Mx = e_1$ and i^* is the index of the root of T_2 .

As remarked earlier, we have that the matrix M is block diagonal, where one block corresponds to the matrix $B = \lambda I - A$, where A is the adjacency matrix of G_n . Furthermore, e_1 is non-zero only in the block corresponding to B . It follows that it suffices to understand the solution $x = B^{-1}e_1$ as padding it with zeroes gives $M^{-1}e_1$.

Similarly to the previous section, we will focus on *layered* vectors x . More formally, we claim there is a layered vector x such that $x = B^{-1}e_1$. That is, all entries of x corresponding to nodes in level i have the same value ϕ_i . Since B is full rank, the solution x to $Bx = e_1$ is unique and thus must equal this layered vector. We thus set out to determine appropriate values ϕ_i .

Similarly to the previous section, we have that choosing ϕ_i 's of the form

$$\phi_i = \alpha \left(\frac{\lambda - \Delta}{4} \right)^i + \beta \left(\frac{\lambda + \Delta}{4} \right)^i,$$

for any $\alpha, \beta \in \mathbb{R}$ and $i = 1, \dots, n+2$ satisfy the recurrence $-2\phi_{i+2} + \lambda\phi_{i+1} - \phi_i = 0$. However, the initial condition we get from $Bx = e_1$ (the first row/equality of the linear system) is different than the previous section. Concretely, the initial condition becomes $\lambda\phi_1 - 2\phi_2 = 1 \Rightarrow \phi_2 = (\lambda/2)\phi_1 - 1/2$. This forces β to be chosen as

$$\begin{aligned} \alpha \cdot \left(\frac{\lambda - \Delta}{4} \right)^2 + \beta \cdot \left(\frac{\lambda + \Delta}{4} \right)^2 &= (\lambda/2) \left(\alpha \cdot \frac{\lambda - \Delta}{4} + \beta \cdot \frac{\lambda + \Delta}{4} \right) - 1/2 \Rightarrow \\ \alpha \cdot (\lambda - \Delta)^2 + \beta \cdot (\lambda + \Delta)^2 &= (2\lambda) (\alpha(\lambda - \Delta) + \beta(\lambda + \Delta)) - 8 \Rightarrow \\ \beta \cdot (\lambda^2 + \Delta^2 + 2\lambda\Delta - 2\lambda(\lambda + \Delta)) &= \alpha \cdot (-\lambda^2 - \Delta^2 + 2\lambda\Delta + 2\lambda(\lambda - \Delta)) - 8 \Rightarrow \\ \beta \cdot (-\lambda^2 + \Delta^2) &= \alpha \cdot (\lambda^2 - \Delta^2) - 8 \Rightarrow \\ -8\beta &= 8\alpha - 8 \Rightarrow \\ \beta &= -\alpha + 1. \end{aligned}$$

Thus ϕ_i 's of the following form, for $1 \leq i \leq n+2$ and $\alpha \in \mathbb{R}$, satisfy the constraints corresponding to T_1

$$\begin{aligned} \phi_i &= \alpha \cdot \left(\left(\frac{\lambda - \Delta}{4} \right)^i - \left(\frac{\lambda + \Delta}{4} \right)^i \right) + \left(\frac{\lambda + \Delta}{4} \right)^i \\ &= \alpha \cdot \left(\frac{\lambda - \Delta}{4} \right)^i \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^i \right) + \left(\frac{\lambda + \Delta}{4} \right)^i. \end{aligned} \quad (12)$$

The tree T_2 puts similar constraints on ϕ_{2n+3-i} for $i = 1, \dots, n+2$, except the root of T_2 gives the initial condition $\lambda\phi_{2n+2} - 2\phi_{2n+1} = 0$ (recall again that we say the root of T_2 is at level $2n+2$). This is precisely the same recurrence as in the previous section. Thus for $1 \leq i \leq n+2$ we have from (10) that for any $\alpha' \in \mathbb{R}$, the following satisfy the constraints of T_2

$$\phi_{2n+3-i} = \alpha' \cdot \left(\frac{\lambda - \Delta}{4} \right)^i \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^i \right). \quad (13)$$

Noting that both (12) and (13) gives a formula for ϕ_{n+1} and ϕ_{n+2} , we get two linear equations in two unknowns, i.e.

$$\alpha \cdot \left(\frac{\lambda - \Delta}{4} \right)^{n+j} \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+j} \right) + \left(\frac{\lambda + \Delta}{4} \right)^{n+j} = \alpha' \cdot \left(\frac{\lambda - \Delta}{4} \right)^{n+3-j} \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+3-j} \right).$$

for $j = 1, 2$. The equations have a unique solution α, α' provided that the two vectors v_j

$$v_j = \left(\left(\frac{\lambda - \Delta}{4} \right)^{n+j} \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+j} \right), \left(\frac{\lambda - \Delta}{4} \right)^{n+3-j} \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+3-j} \right) \right)$$

with $j = 1, 2$ are linearly independent. To see that they are linearly independent, we compare the ratio $r_1 = v_1(1)/v_2(1)$ of the first coordinate v_1 and v_2 to the ratio $r_2 = v_1(2)/v_2(2)$ of the second coordinate. We have that v_1 and v_2 are linearly independent if these ratios are distinct. The ratios of the coordinates are

$$r_1 = \left(\frac{\lambda - \Delta}{4} \right)^{-1} \frac{\left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1} \right)}{\left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2} \right)}, r_2 = \left(\frac{\lambda - \Delta}{4} \right) \frac{\left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2} \right)}{\left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1} \right)}.$$

We thus have $r_1 = r_2^{-1}$, implying linear independence whenever $|r_2| \neq 1$. To argue that this is the case, we prove the following auxiliary results using simple approximations of $(1+x)^a$

Claim 1. For $i \leq n+2 \leq \gamma^{-1/2}/16$ and $0 < \gamma \leq 1/64$, we have $\Delta \leq 4\sqrt{\gamma}$,

1.

$$0 < \frac{2\Delta}{\lambda + \Delta} < \frac{2\Delta}{\lambda - \Delta} < \frac{1}{2(n+2)},$$

2.

$$1 + \frac{i\Delta}{\lambda - \Delta} \leq \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^i \leq 1 + \frac{4i\Delta}{\lambda - \Delta}.$$

3.

$$1 - \frac{4i\Delta}{\lambda + \Delta} \leq \left(\frac{\lambda - \Delta}{\lambda + \Delta} \right)^i \leq 1 - \frac{i\Delta}{\lambda + \Delta}.$$

4.

$$1 + \frac{1}{2(n+1)} \leq \frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}} \leq 1 + \frac{4}{n+1}.$$

From Claim 1 point 4., $\lambda - \Delta \leq \lambda = \sqrt{8} + \gamma$, $n+2 \leq \gamma^{-1/2}/16$, $\gamma \leq 1/64$ and n large enough, we get

$$0 < r_2 \leq \frac{\sqrt{8} + 1/64}{4} \cdot \left(1 + \frac{4}{n+1} \right) < 1,$$

implying linear independence and thus existence of a unique solution α, α' . We defer the proof of Claim 1 to Section 4.3 as it consists of careful, but simple, calculations.

We now derive a number of properties of this unique choice of α and α' . For this, we need one last auxiliary result

Claim 2. For $n+2 \leq \gamma^{-1/2}/16$ and $0 < \gamma \leq 1/64$, we have

$$-1 - \frac{2}{n+1} \leq \alpha \left(\left(\frac{\lambda - \Delta}{\lambda + \Delta} \right)^{n+1} - 1 \right) \leq -1 - \frac{1}{4(n+1)}.$$

We again defer the proof of Claim 2 to Section 4.3.

Our goal is now to bound all terms ϕ_i in terms of ϕ_{2n+2} as ϕ_{2n+2} is the value of the entry of x corresponding to the root of T_2 . We do this in two steps. First, we relate all ϕ_i to ϕ_{n+1} as both (12) and (13) gives a formula for ϕ_{n+1} . Using the relationship between ϕ_{2n+2} and ϕ_{n+1} then indirectly relates all ϕ_i to ϕ_{2n+2} .

For $i \leq n+1$, we relate ϕ_{2n+3-i} to ϕ_{n+1} directly from (13), giving

$$\frac{\phi_{2n+3-i}}{\phi_{n+1}} = \left(\frac{\lambda - \Delta}{4} \right)^{i-n-2} \cdot \frac{\left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^i - 1}{\left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2} - 1}.$$

From Claim 1, this implies

$$\left(\frac{\lambda - \Delta}{4} \right)^{i-n-2} \frac{i}{4(n+2)} \leq \frac{|\phi_{2n+3-i}|}{|\phi_{n+1}|} \leq \left(\frac{\lambda - \Delta}{4} \right)^{i-n-2} \frac{4i}{n+2}. \quad (14)$$

To bound the terms ϕ_i with $i \leq n+1$, we get from (12) that

$$\frac{\phi_i}{\phi_{n+1}} = \left(\frac{\lambda + \Delta}{4}\right)^{i-n-1} \cdot \frac{\alpha \left(\left(\frac{\lambda - \Delta}{\lambda + \Delta} \right)^i - 1 \right) + 1}{\alpha \left(\left(\frac{\lambda - \Delta}{\lambda + \Delta} \right)^{n+1} - 1 \right) + 1}. \quad (15)$$

Using Claim 2, we conclude

$$\begin{aligned} \frac{|\phi_i|}{|\phi_{n+1}|} &\leq \left(\frac{\lambda + \Delta}{4}\right)^{i-n-1} \cdot \frac{\left| \alpha \left(\left(\frac{\lambda - \Delta}{\lambda + \Delta} \right)^i - 1 \right) \right| + 1}{(4(n+1))^{-1}} \\ &\leq 4(n+1) \cdot \left(\frac{\lambda + \Delta}{4}\right)^{i-n-1} \cdot \left(\left| \alpha \left(\left(\frac{\lambda - \Delta}{\lambda + \Delta} \right)^{n+1} - 1 \right) \right| + 1 \right) \\ &\leq 12(n+1) \cdot \left(\frac{\lambda + \Delta}{4}\right)^{i-n-1}. \end{aligned} \quad (16)$$

Note here that it was crucial that our bound in Claim 2 was very tight since the denominator in (15) is very close to zero.

From (14) with $i = 1$, we conclude

$$|\phi_{n+1}| \leq |\phi_{2n+2}| 4(n+2) \left(\frac{\lambda - \Delta}{4} \right)^{n+1}. \quad (17)$$

Inserting (17) into (14), we now get for $i \leq n+2$ that:

$$|\phi_{2n+3-i}| \leq 4(n+2)|\phi_{2n+2}| \left(\frac{\lambda - \Delta}{4} \right)^{i-1} \frac{4i}{n+2} = 16i|\phi_{2n+2}| \left(\frac{\lambda - \Delta}{4} \right)^{i-1}.$$

Similarly, inserting (17) into (16), we get

$$|\phi_i| \leq 4(n+2)|\phi_{2n+2}| 12(n+1) \left(\frac{\lambda + \Delta}{4} \right)^i \leq 48(n+2)^2 |\phi_{2n+2}| \left(\frac{\lambda + \Delta}{4} \right)^i.$$

Using that there are 2^{i-1} nodes at level i and $2n+3-i$, we finally get that

$$\begin{aligned}
\|x\|^2 &= \sum_{i=1}^{n+1} 2^{i-1} (\phi_i^2 + \phi_{2n+3-i}^2) \\
&\leq \sum_{i=1}^{n+1} 2^{i-1} \left((16i)^2 \left(\frac{\lambda - \Delta}{4} \right)^{2i-2} + 48^2 (n+2)^4 \left(\frac{\lambda + \Delta}{4} \right)^{2i} \right) \phi_{2n+2}^2 \\
&= O \left(n^4 \phi_{2n+2}^2 \sum_{i=1}^{n+1} 2^i \left(\frac{\lambda + \Delta}{4} \right)^{2i} \right) \\
&= O \left(n^4 \phi_{2n+2}^2 \sum_{i=1}^{n+1} 2^i \left(\frac{\lambda^2 + \Delta^2 + 2\lambda\Delta}{16} \right)^i \right) \\
&= O \left(n^4 \phi_{2n+2}^2 \sum_{i=1}^{n+1} 2^i \left(\frac{2(8 + 2\sqrt{8}\gamma + \gamma^2) - 8 + 2(\sqrt{8} + \gamma)4\sqrt{\gamma}}{16} \right)^i \right) \\
&= O \left(n^4 \phi_{2n+2}^2 \sum_{i=1}^{n+1} 2^i \left(\frac{8 + 48\sqrt{\gamma}}{16} \right)^i \right) \\
&= O \left(n^4 \phi_{2n+2}^2 \sum_{i=1}^{n+1} 2^i \left(\frac{1}{2} (1 + 6\sqrt{\gamma}) \right)^i \right) \\
&= O(n^5 \phi_{2n+2}^2 (1 + 6\sqrt{\gamma})^n) \\
&= O(n^5 \phi_{2n+2}^2 e^{6\sqrt{\gamma}n}).
\end{aligned}$$

For $n+2 \leq \gamma^{-1/2}/16$, this is $O(n^5 \phi_{2n+2}^2)$, implying $\phi_{2n+2}^2 = \Omega(n^{-5} \|x\|^2)$. Since ϕ_{2n+2} is the value x_{i^*} of the root i^* of T_2 , this completes the proof.

4.3 Auxiliary Results

In this section, we prove the two auxiliary claims in Claim 1 and Claim 2. The first claim uses simple approximations of $(1+x)^a$ without any particularly novel ideas.

Proof of Claim 1. Using a Taylor series, we have for $0 \leq x < 1$ that

$$\begin{aligned}
1+x &= \exp \left(\sum_{n=1}^{\infty} (-1)^{n+1} x^n / n \right) \\
&\geq \exp(x - x^2/2) \\
&\geq \exp(x/2).
\end{aligned}$$

At the same time, it holds for all x that $1+x \leq e^x$. Now observe that $\Delta = \sqrt{(\sqrt{8} + \gamma)^2 - 8} = \sqrt{2\sqrt{8}\gamma + \gamma^2}$. Thus $\sqrt{\gamma} \leq \Delta \leq 4\sqrt{\gamma}$ when $\gamma \leq 1$. This implies for $\gamma \leq 1/64$ that

$$\frac{2\Delta}{\lambda - \Delta} \leq \frac{8\sqrt{\gamma}}{\sqrt{8} - 4\sqrt{\gamma}} \leq \frac{8\sqrt{\gamma}}{\sqrt{8} - 1/2} \leq 8\sqrt{\gamma}. \quad (18)$$

For integer $i \leq \gamma^{-1/2}/8$, we therefore have that $\left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^i = \left(1 + \frac{2\Delta}{\lambda - \Delta} \right)^i$ satisfies

$$1 + \frac{i\Delta}{\lambda - \Delta} \leq \exp \left(i \cdot \frac{\Delta}{\lambda - \Delta} \right) \leq \left(1 + \frac{2\Delta}{\lambda - \Delta} \right)^i \leq \exp \left(i \cdot \frac{2\Delta}{\lambda - \Delta} \right) \leq 1 + \frac{4i\Delta}{\lambda - \Delta}. \quad (19)$$

For $0 \leq x < 1/2$, we also have $1 - x \leq e^{-x}$ and $1 - x = \exp(-\sum_{n=1}^{\infty} x^n/n) \geq \exp(-\sum_{n=1}^{\infty} x(1/2)^{n-1}) \geq \exp(-2x)$. Since $0 < 2\Delta/(\lambda + \Delta) \leq 2\Delta/(\lambda - \Delta) \leq 8\sqrt{\gamma}$, we thus conclude for $i \leq \gamma^{-1/2}/16$ that $\left(\frac{\lambda-\Delta}{\lambda+\Delta}\right)^i = \left(1 - \frac{2\Delta}{\lambda+\Delta}\right)^i$ satisfies

$$1 - \frac{4i\Delta}{\lambda + \Delta} \leq \exp\left(-4i \cdot \frac{\Delta}{\lambda + \Delta}\right) \leq \left(1 - \frac{2\Delta}{\lambda + \Delta}\right)^i \leq \exp\left(-i \cdot \frac{2\Delta}{\lambda + \Delta}\right) \leq 1 - \frac{i\Delta}{\lambda + \Delta}.$$

We finally bound the ratio

$$\frac{1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+2}}{1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}} = \frac{1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1} - \frac{2\Delta}{\lambda-\Delta} \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}}{1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}} = 1 + \frac{\frac{2\Delta}{\lambda-\Delta} \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}}{\left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1} - 1}.$$

From (19) and $n + 2 \leq \gamma^{-1/2}/16$, we have

$$\frac{\frac{2\Delta}{\lambda-\Delta} \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}}{\left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1} - 1} \geq \frac{\frac{2\Delta}{\lambda-\Delta}}{\left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1} - 1} \geq \frac{\frac{2\Delta}{\lambda-\Delta}}{\frac{4(n+1)\Delta}{\lambda-\Delta}} = \frac{1}{2(n+1)}.$$

From (19), (18) and $n + 2 \leq \gamma^{-1/2}/16$ we similarly get

$$\frac{\frac{2\Delta}{\lambda-\Delta} \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}}{\left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1} - 1} \leq \frac{\frac{2\Delta}{\lambda-\Delta} \left(1 + \frac{4(n+1)}{\lambda-\Delta}\right)}{\frac{(n+1)\Delta}{\lambda-\Delta}} \leq \frac{2}{n+1} + \frac{8\Delta}{\lambda-\Delta} \leq \frac{2}{n+1} + 32\sqrt{\gamma} \leq \frac{4}{n+1}.$$

Thus

$$1 + \frac{1}{2(n+1)} \leq \frac{1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+2}}{1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}} \leq 1 + \frac{4}{n+1}.$$

□

We next proceed to give the proof of Claim 2. Their key idea here is to consider the ratio ϕ_{n+1}/ϕ_{n+2} using both (12) and (13).

Proof of Claim 2. Consider the ratio ϕ_{n+1}/ϕ_{n+2} . Using (12), this ratio equals

$$\frac{\phi_{n+1}}{\phi_{n+2}} = \frac{\left(\frac{\lambda-\Delta}{4}\right)^{n+1} \left(\alpha \left(1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}\right) + \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}\right)}{\left(\frac{\lambda-\Delta}{4}\right)^{n+2} \left(\alpha \left(1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+2}\right) + \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+2}\right)}.$$

This implies

$$\frac{\phi_{n+1}}{\phi_{n+2}} \cdot \left(\frac{\lambda-\Delta}{4}\right) \left(\alpha \left(1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+2}\right) + \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+2}\right) = \left(\alpha \left(1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}\right) + \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}\right).$$

Using (13), we also have

$$\frac{\phi_{n+1}}{\phi_{n+2}} = \frac{\lambda - \Delta}{4} \cdot \frac{1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+2}}{1 - \left(\frac{\lambda+\Delta}{\lambda-\Delta}\right)^{n+1}}$$

Inserting this above and rearranging terms gives

$$\alpha \left(1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1} \right) \left(\left(\frac{\lambda - \Delta}{4} \right)^2 \left(\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}} \right)^2 - 1 \right) = \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1} \left(1 - \left(\frac{\lambda + \Delta}{4} \right) \left(\frac{\lambda - \Delta}{4} \right) \frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}} \right). \quad (20)$$

Rearranging terms and using $\lambda^2 - \Delta^2 = 8$ gives

$$\begin{aligned} \alpha \left(\left(\frac{\lambda - \Delta}{\lambda + \Delta} \right)^{n+1} - 1 \right) &= \frac{1 - \frac{1}{2} \cdot \frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}}}{\left(\frac{\lambda - \Delta}{4} \right)^2 \left(\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}} \right)^2 - 1} \\ &= \frac{1}{2} \cdot \frac{1}{\left(\frac{\lambda - \Delta}{4} \right)^2 \left(\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}} \right) - \left(\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}} \right)} \end{aligned} \quad (21)$$

Using Claim 1 point 4. to bound the ratio

$$\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}} \geq 1 + \frac{1}{2(n+1)},$$

the denominator of (21) is at least

$$\left(\frac{\lambda - \Delta}{4} \right)^2 \left(\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}} \right) - \left(\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+1}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta} \right)^{n+2}} \right) \geq \left(\frac{\lambda - \Delta}{4} \right)^2 \left(1 + \frac{1}{2(n+1)} \right) - 1. \quad (22)$$

We now observe that

$$\begin{aligned} \left(\frac{\lambda - \Delta}{4} \right)^2 &= \frac{\lambda^2 + \Delta^2 - 2\lambda\Delta}{16} \\ &= \frac{2(8 + 2\sqrt{8}\gamma + \gamma^2) - 8 - 2\lambda\Delta}{16} \\ &\geq \frac{1}{2} + \frac{4\sqrt{8}\gamma + 2\gamma^2 - 24\sqrt{\gamma}}{16} \\ &> \frac{1}{2} - \sqrt{\gamma} \\ &\geq \frac{1}{2} - \frac{1}{16(n+2)}. \end{aligned}$$

Continuing from (22), we have that the denominator of (21) is at least

$$\left(\frac{1}{2} - \frac{1}{16(n+2)} \right) \left(1 + \frac{1}{2(n+1)} \right) - 1 \geq -\frac{1}{2} + \frac{1}{4(n+1)} - \frac{1}{16(n+1)} - \frac{1}{32(n+1)^2} \geq -\frac{1}{2} + \frac{1}{8(n+1)}.$$

We may also upper bound the denominator as

$$\begin{aligned}
\left(\frac{\lambda - \Delta}{4}\right)^2 \left(\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta}\right)^{n+2}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta}\right)^{n+1}}\right) - \left(\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta}\right)^{n+1}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta}\right)^{n+2}}\right) &\leq \\
\left(\frac{\lambda - \Delta}{4}\right)^2 - \left(\frac{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta}\right)^{n+1}}{1 - \left(\frac{\lambda + \Delta}{\lambda - \Delta}\right)^{n+2}}\right) &\leq \\
\frac{1}{2} - \left(1 + \frac{1}{2(n+1)}\right)^{-1} &= \\
\frac{1}{2} - \frac{2(n+1)}{2(n+1)+1} &= \\
\frac{1}{2} - 1 + \frac{1}{2(n+1)+1} &\leq \\
-\frac{1}{2} + \frac{1}{2(n+1)}. &
\end{aligned}$$

Using these bounds in (21) we conclude

$$\begin{aligned}
\alpha \left(\left(\frac{\lambda - \Delta}{\lambda + \Delta} \right)^{n+1} - 1 \right) &\leq \frac{1}{-1 + \frac{1}{4(n+1)}} \\
&= - \left(\frac{1}{1 - \frac{1}{4(n+1)}} \right) \\
&= - \left(1 + \frac{\frac{1}{4(n+1)}}{1 - \frac{1}{4(n+1)}} \right) \\
&\leq -1 - \frac{1}{4(n+1)}.
\end{aligned}$$

and

$$\begin{aligned}
\alpha \left(\left(\frac{\lambda - \Delta}{\lambda + \Delta} \right)^{n+1} - 1 \right) &\geq \frac{1}{-1 + \frac{1}{n+1}} \\
&= - \left(\frac{1}{1 - \frac{1}{n+1}} \right) \\
&= - \left(1 + \frac{\frac{1}{n+1}}{1 - \frac{1}{n+1}} \right) \\
&\geq -1 - \frac{2}{n+1}.
\end{aligned}$$

□

Acknowledgment

Kasper Green Larsen is co-funded by a DFF Sapere Aude Research Leader Grant No. 9064-00068B by the Independent Research Fund Denmark and co-funded by the European Union (ERC, TUCLA, 101125203).

Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.

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