Continuous Time Quantum Walks in finite Dimensions

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PACS numbers: 05.10.Cc,03.67.Ac, 05.40.Fb

Quantum walks present one of the frameworks for which quantum computing can satisfy its promise to provide a significant speed-up over classical computation. Grover [1] has shown that a quantum walk can locate an entry in an unordered list of $N$ sites in a time that scales as $\sim \sqrt{N}$, a quadratic speed-up over classical search algorithms. However, that finding was based on a list in which all sites are interconnected with each other, thus, raising the question regarding the impact of geometry on quantum search. Our results are consistent with those of Childs and Goldstone [Phys. Rev. A 70 (2004), 022314] for lattices of integer dimension, where $d = d_L = d_s$. For general fractals, we find that the Grover limit of quantum search can be obtained whenever $d_s > 4$. This complements the recent discussion of mean-field (i.e., $d_s \to \infty$) networks by Chakraborty et al. [Phys. Rev. Lett. 116 (2016), 100501] showing that for all those networks spatial search by quantum walk is optimal.

Here, we generalize those results to arbitrary real (fractal) dimensions $d$. Fractals generally possess both a fractal dimension $d_f$ and a spectral dimension $d_s$ that can vary independently to characterize their geometry [9], while for regular lattices $d_f = d_s = d$. Scaling as well as exact renormalization group (RG) arguments show that the spectral dimension $d_s$ of the lattice Laplacian controls the ability of CTQW to saturate the Grover limit generally, even for cases where $d_f \neq d_s$.

Certain graphs with fractal dimensions have been considered previously for search with CTQW [10]. The fractals chosen there include dual Sierpinski gaskets, T-fractals, Cayley trees, and Cartesian products between Euclidean lattices and dual Sierpinski gaskets, with a variety of fractal and spectral dimensions. Based on numerical simulations, it was suggested that whether CTQW provides quadratic speedup is determined together by a spectral dimension larger than 4 and by the overlaps of the initial state with the ground and first excited state of the Hamiltonian. These overlaps undergo a critical transition near the closest “gap” between both levels, controlled by the choice of $\gamma$ in Eq. (1). In this paper, we explicitly relate the transition in $\gamma$ to (derivatives of) the Laplacian determinant using a spectral $\zeta$-function. Using exact RG [11], we have shown elsewhere that the asymptotic scaling of the Laplacian determinant is described uniquely in terms of $d_s$.

The continuous time quantum walk on a graph is determined by the Schrödinger equation evolving in a Hilbert space spanned by the $N$-position site-basis $|x\rangle$,

$$i \frac{d\Psi_x(t)}{dt} = \sum_y \mathcal{H}_{xy} \Psi_y(t),$$

where $\Psi_x(t) = \langle x|\Psi(t)\rangle$ is the complex amplitude at site $x$, and $\mathcal{H}$ is the Hamiltonian defined in Eq. (1). The search typically evolves from an initial state that is prepared as the uniform superposition over all sites $|1\rangle$, $|s\rangle = \frac{1}{\sqrt{N}} \sum_x |x\rangle$. The complete graph is a special

$$\mathcal{H} = \gamma \mathcal{L} - |w\rangle \langle w|,$$

where $\mathcal{L}$ is the Laplacian matrix, and $|w\rangle \langle w|$ is the projection operator (the oracle) for some target site $w$. With that, a quadratic speedup for quantum search has been shown for high dimensional graphs such as the complete graph [2] and the hypercube [3, 4]. Recently, it has been proven also to be optimal on Erdős-Rényi graphs with $N$ sites as long as the existence probability for an edge between any two sites is $p \geq \log^{3/2} N/N$ or the graphs are regular, i.e., they have the same degree for every site [5]. However, Childs and Goldstone [6] have shown that such a quantum search can reach the Grover limit of quantum walks on lattices in dimensions $d > 4$ only, while in $d = 4$, the running time to achieve a success probability of order 1 is $O(\sqrt{N} \log^{3/2} N)$, with increasing deviations from $\sqrt{N}$-scaling for $d = 3$ and 2. In contrast, a discrete-time, coined version of a quantum walk has been proposed by which quantum search falls short of the Grover limit in $d = 2$ only by logarithmic factors [7, 8]. A better understanding of this discrepancy, its origin and potential remedies, is of considerable interest.

We consider the quantum search problem with a continuous time quantum walk for networks of finite spectral dimension $d_s$ of the network Laplacian. For general networks of fractal (integer or non-integer) dimension $d_f$, for which in general $d_f \neq d_s$, it suggests that $d_s$ is the scaling exponent that determines the computational complexity of the search. Our results are consistent with those of Childs and Goldstone [Phys. Rev. A 70 (2004), 022314] for lattices of integer dimension, where $d = d_f = d_s$. For general fractals, we find that the Grover limit of quantum search can be obtained whenever $d_s > 4$. This complements the recent discussion of mean-field (i.e., $d_s \to \infty$) networks by Chakraborty et al. [Phys. Rev. Lett. 116 (2016), 100501] showing that for all those networks spatial search by quantum walk is optimal.
case of CTQW, where it suffices to consider the subspace spanned by \(|s\rangle\) and \(|w\rangle\) on which the Hamiltonian acts nontrivially. At \(\gamma N = 1\), the ground and first excited state are respectively \(|w\rangle \pm |s\rangle\) \(\sqrt{2}\) with a energy gap of \(2/\sqrt{N}\). The search Hamiltonian achieves success by driving the system from state \(|s\rangle\) to \(|w\rangle\) with a transition probability \(H_{s,w} = \langle\langle w|e^{-i\hat{H}t}|s\rangle\rangle^2 = \sin t/\sqrt{N}\) that reaches unity first at time \(t = \frac{\pi}{2}\sqrt{N}\). For a general geometry, the ground and first excited state are more complicate than a superposition of \(|s\rangle\) and \(|w\rangle\). Yet, the objective of CTQW remains two-fold: (1) find a critical value \(\gamma = \gamma_c\) such that the overlaps between \(|s\rangle\) as well as \(|w\rangle\) and the ground and first excited state are substantial, and (2) ascertain that at this critical point the Hamiltonian drives a transition from \(|s\rangle\) to \(|w\rangle\) in a time \(t \sim 1/(E_1 - E_0) \sim \sqrt{N}\).

We denote eigenvalues and normalized orthogonal eigenstates for \(\mathcal{H}\) and \(\mathcal{L}\) respectively as \(\{E_i, |\psi_i\rangle\}\) and \(\{\lambda_i, |\phi_i\rangle\}\) for \(0 \leq i < N\). Note that the initial state \(|s\rangle = |\phi_0\rangle\) is, in fact, the lowest eigenstate of the Laplacian with \(\mathcal{L}|s\rangle = 0\), i.e., the associated eigenvalue is \(\lambda_0 = 0\), while all other Laplacian eigenvalues are positive. Ref. \[6\] has derived a spectral function for \(\mathcal{H}\) in terms of the Laplacian eigenstates that is convenient for the discussion of translationally invariant lattices:

\[
F(E) = \left\langle w \right| \frac{1}{\sqrt{\mathcal{L} - E}} \left| w \right\rangle = \sum_{i=0}^{N-1} \frac{|w_i|^2}{\lambda_i - E}. \tag{3}
\]

The condition on the Hamiltonian eigenvalues,

\[
F(E_i) = 1, \tag{4}
\]

is provided in terms of the Laplacian eigenvalues. From the spectral function, one can derive the overlap of any eigenstate with the initial state as

\[
|\left\langle s \right| \psi_i \rangle|^2 = \frac{1}{N E_i^2 F'(E_i)}. \tag{5}
\]

The key objective of a quantum search concerns optimizing the transition amplitude between the initial state and the target site,

\[
\left\langle w \left| e^{-i\hat{H}t} \right| s \right\rangle = -\frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} e^{iE_i t} E_i F'(E_i). \tag{6}
\]

The Hamiltonian \(\mathcal{H}\) (i.e., \(\gamma\)) has to be optimized such that this amplitude reaches a finite magnitude in the shortest amount of time in the limit of large \(N\).

For regular lattices, the overlap of the eigenstates of the Laplacian with any member of the site basis, in particular \(|w\rangle\), is uniform and independent of \(w\). However, this is generally not true for fractals \[15\]; such heterogeneity could lead to a large variability in the "findability" of a significant number of ill-placed sites \(w\) \[16\]. We have to assume (and will demonstrate below) that at typical sites \(w\) of some fractal networks, the overlaps with eigenvectors of the Laplacian still satisfy

\[
|\left\langle w \right| \phi_i \rangle|^2 \sim \frac{1}{N}, \tag{7}
\]

as they are for the Fourier modes of the lattice. With that, and also remembering that \(\lambda_0 = 0\), Eq. (3) can be rewritten as

\[
F(E) \sim -\frac{1}{N} + \frac{1}{\gamma} I_1 + \frac{1}{N} \sum_{i=1}^{N-1} \frac{E}{\gamma \lambda_i (\gamma \lambda_i - E)}, \tag{8}
\]

defining the spectral \(\zeta\)-function \[17, 18\]

\[
I_j \sim \frac{1}{N} \sum_{i=1}^{N-1} \left( \frac{1}{\lambda_i} \right)^j, \tag{9}
\]

which will play a central role in the analysis. These quantities have been considered before, in particular by Ref. \[6\], to examine search by CTQW on regular lattices, or in Ref. \[10\] for fractals. In Ref. \[10\], it was assumed that Eq. (9) requires complete knowledge of the entire Laplacian spectrum, which is rarely achievable. Here, we want to point out that \(I_j\) can be reduced to the evaluation of the determinant of \(\mathcal{L}\) and derivatives thereof. Using the fact that

\[
\sum_{i=1}^{N-1} \ln \lambda_i = \ln \left[ \frac{1}{\gamma} \prod_{i=0}^{N-1} (\lambda_i + \epsilon) \right]_{\epsilon \to 0},
\]

we have obtained in Ref. \[14\] asymptotic behavior of the spectral \(\zeta\)-function defined in Eq. (9) as

\[
I_j \sim \left( \frac{\partial}{\partial \epsilon} \right)^j \left[ \frac{1}{\epsilon} \det (\mathcal{L} + \epsilon) \right]_{\epsilon \to 0} \tag{10}
\]

\[
\sim \begin{cases} N \frac{2^j - 1}{j}, & d_s < 2j, \
\text{const}, & d_s > 2j. \end{cases} \tag{11}
\]

for fractal networks with the spectral dimension \(d_s\). Thus, \(d_s\) becomes the key characteristic for any network, such as those fractals for which \(d = d_f \neq d_s\), that determines whether the Grover limit can be achieved. For example, as observed in Ref. \[6\], this quantum search becomes optimal for lattices of any dimension when there is a phase transition in the overlaps \(|\langle s | \psi_0 \rangle|^2\) and \(|\langle s | \psi_1 \rangle|^2\), of which the former rises while the latter declines for increasing \(\gamma\). This critical point occurs for

\[
\gamma \sim \gamma_c = I_1. \tag{12}
\]

Accordingly, we find for general fractal networks that

\[
\gamma_c \sim \begin{cases} N \frac{2^j - 1}{j}, & d_s < 2, \
\text{const}, & d_s > 2. \end{cases} \tag{13}
\]
To obtain the runtime complexity for the quantum search, we have to distinguish the following cases: For $d_s > 4$, according to Eq. (10), both $I_{1,2}$ remain constant. It is then self-consistent to consider the spectral function in Eq. (8) for energies $|E| \ll \gamma_c \lambda_1$, which applies to both the ground state $E_0$ and the first excited state $E_1$ of $\mathcal{H}$ near the optimal (“critical”) $\gamma_c$. Expanding the remaining sum in Eq. (8) to leading order in $E$ yields

$$F(E) \sim -\frac{1}{NE} + \frac{1}{\gamma} I_1 + \frac{E}{\gamma^2} I_2 + \ldots, \quad (|E| \ll \gamma_c \lambda_1),$$

(14)

Since $F(E_{0,1}) = 1$ from the eigenvalue condition in Eq. (4), we obtain a consistent balance to leading and sub-leading order only for $\gamma = \gamma_c = I_1$, thereby validating Eq. (12), and for

$$E_{0,1} \sim \pm \frac{1}{\sqrt{N}} \frac{I_1}{\sqrt{I_2}} = O\left(N^{-\frac{1}{2}} \right).$$

(15)

Then, the derivative of Eq. (14) provides $F'(E_{0,1}) \sim 2I_2/I_1^2$ such that according to Eq. (5) the initial state $|s\rangle$ overlaps with equal and finite weight with both, ground state and first excited state:

$$|\langle s | \psi_{0,1}\rangle|^2 \sim \frac{1}{2}.$$  

(16)

As $E_i > \gamma_c \lambda_1$ for all $i \geq 2$, higher energy eigenstates do not contribute for large $N$, and we obtain from the first two terms of the transition amplitude in Eq. (6),

$$\left|\langle w | e^{i \mathcal{H}_1 t} | s\rangle\right|^2 \sim \frac{1}{N} \left| \frac{e^{i E_{0,t}}}{E_0 F'(E_0)} + \frac{e^{i E_{1,t}}}{E_1 F'(E_1)} \right|^2,$$

(17)

$$\sim \frac{I_2^2}{I_1^2} \sin^2 \left(\frac{2 I_1 \sqrt{t}}{\sqrt{I_2} \sqrt{N}}\right).$$

(18)

Thus, the transition probability oscillates and reaches its first maximum at a time

$$t = t_{\text{opt}} \sim \frac{\sqrt{I_2}}{I_1} \sqrt{N} = O\left(N^{\frac{1}{2}} \right),$$

(19)

at which point the transition probability becomes

$$p_{\text{opt}} = \left|\langle w | e^{i \mathcal{H}_{\text{opt}} t} | s\rangle\right|^2 \sim \frac{I_2^2}{I_1^2} = O(1).$$

(20)

Finally, to find the targeted site $w$ with a probability of order unity, we need to run the quantum search $\sim 1/p_{\text{opt}}$ times, each for a time of $t_{\text{opt}}$ at which a measurement must be executed. Thus, the runtime complexity for a successful search is given by

$$\frac{t_{\text{opt}}}{p_{\text{opt}}} \sim \left(\frac{I_2}{I_1}\right)^{\frac{3}{2}} \sqrt{N} = O\left(N^{\frac{3}{2}} \right), \quad (d_s > 4).$$

(21)

For case $d_s = 4$, $I_1$ remains constant while $I_2 \sim \ln N$ acquires a logarithmic correction in the limit $d_s \to 4$. With that, the analysis of the previous case remains applicable, although the condition $|E| \ll \gamma_c \lambda_1$ is merely logarithmically satisfied. Thus, we obtain from Eq. (21) in this interpretation that

$$\frac{t_{\text{opt}}}{p_{\text{opt}}} = O\left(N\frac{3}{2} \ln^2 N \right), \quad (d_s = 4).$$

(22)
For case $2 < d_s < 4$, $I_1$ remains constant while $I_2 \sim N^{-\frac{d_s}{d_s-1}}$. However, by Eq. (15), this would imply $E_{0,1} \sim N^{-\frac{d_s}{d_s-1}}$, which would violate the condition of $E_{0,1} \ll \gamma_\epsilon \lambda_1$ where $\lambda_1 \sim \Lambda N^{-\frac{d_s}{d_s-1}}$. As a consequence, the expansion in Eq. (14) is no longer valid and we have to reconsider Eq. (8) anew at $\gamma = \gamma_\epsilon \sim I_1$, but with $\gamma_\epsilon \lambda_1 \sim E_{0,1} = e_{0,1} I_1 \Lambda N^{-\frac{d_s}{d_s-1}}$. Then, Eq. (8) provides

$$F(E_{0,1}) \sim \frac{1}{I_1 \Lambda e_{0,1}} N^{\frac{d_s}{d_s-1}} + \frac{e_{0,1}}{I_1 \Lambda (1 - e_{0,1})} N^{\frac{d_s}{d_s-1}} + \ldots,$$

where the two leading corrections cancel self-consistently with a negative (positive) solution for $e_{0,1} (e_{0,1} \Lambda)$. Then, $E_{0,1} F'(E_{0,1}) \sim N^{\frac{d_s}{d_s-1}}$, such that by Eq. (18), the transition probability diminishes for falling $d_s$ and is at best

$$|\langle w | e^{i\mathcal{H}_t} | s \rangle|^2 \leq \frac{1}{N} \left| \frac{1}{E_0 F'(E_0)} \right|^2 \sim N^{1 - \frac{d_s}{d_s-1}}.$$

In turn, to accomplish any significant change in this transition amplitude requires at time of at least $t_{\text{opt}} \geq \frac{1}{p_{\text{opt}}} \sim N^{\frac{d_s}{d_s-1}}$, which for $d_s \rightarrow 2$ also reproduces the known conclusion for the 2d regular lattice, up to logarithmic corrections.

Finally, we confirm numerically the assumption in Eq. (7) that for typical vertices $w$, the overlap with Laplacian eigenvectors scales as $|\langle w | \phi_i \rangle|^2 \sim 1/N$. For example, in Ref. [14], we have considered the Laplacians for fractal networks in the Migdal-Kadanoff renormalization group (MKRG) [12, 13], which mimic the properties of regular networks in the Migdal-Kadanoff renormalization group (MKRG) [12, 13], which mimic the properties of regular networks. However, since they constitute by far the largest fraction and are the most uniform, sites in the highest level of the hierarchy exhibit what can be considered as the typical behavior. In Fig. 2, we have plotted the overlaps for searched-for sites $w$ with all eigenvectors $|\phi_i\rangle$, $0 \leq i < N$ of the respective Laplacian but averaged separately over all $w$ in the highest, 2nd-highest, and 3rd-highest levels of the hierarchy for MKRG networks of $b = 2$ after $g = 6$ generations of the hierarchy, and for $b = 3$ after $g = 5$ generation. For sites $w$ in the highest level, the overlaps are essentially uniform and satisfy Eq. (7) for all $i$. For $w$ on lower levels, their overlaps with an increasing number of eigenvectors related to the largest eigenvalues $\lambda_i$ outright vanishes, while the non-vanishing overlaps remain with few

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Figure 2: Plot of the overlaps $|\langle w | \phi_i \rangle|^2$ in MKRG for the searched-for sites $w$ with the Laplacian eigenvectors $\phi_i$ as a function of $i$, ordered such that respective eigenvalues satisfy $\lambda_i \leq \lambda_{i'}$ for any two indices $i \leq i'$. The MKRG used here [19] rescales length by $l = 2$ with (a) $b = 2$ and (b) $b = 3$ branches in each RG-step for an effective dimension $d = 1 + \log b$ of (a) $d = 2$ and (b) $d = 2.585 \ldots$. The RG has been iterated for $g = 6$ generations in the hierarchy in (a), forming a lattice of $N = 2 + \frac{b}{2^{d-1}} (2b)^9 = 2732$ sites, and in (b) for $g = 5$ with $N = 4667$ sites. In the top panel of both, (a) and (b), the overlaps (rescaled by a factor of $N$) were averaged over all sites $w$ in the highest hierarchical level $g$, in the middle panel overlaps were averaged only over those $w$ in level $g - 1$, and in the respective bottom panel for level $g - 2$. Note that every level the number of sites increases by a factor of $\sim 2b$, such that the vast majority of all sites $w$ are typically located in these highest levels of the hierarchy. For those, these plots show that indeed $N |\langle w | \phi_i \rangle|^2 \sim 1$, typically, as assumed in Eq. (7), although these overlaps progressively vanish for those $w$ in lower levels for eigenvectors of larger index $i$. 

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Figure 2 (continued): Plots of the overlaps $|\langle w | \phi_i \rangle|^2$ in MKRG for the searched-for sites $w$ with the Laplacian eigenvectors $\phi_i$. For the majority of all sites $w$, in the highest level of the hierarchy, and for those, the overlaps are essentially uniform and satisfy Eq. (7) for all $i$. For $w$ on lower levels, their overlaps with an increasing number of eigenvectors related to the largest eigenvalues $\lambda_i$ outright vanishes, while the non-vanishing overlaps remain with few
exceptions uniform and $O(1/N)$. This fact suggests that the runtime complexity differs mildly between sites $w$ in different hierarchies. For our purpose here, we conclude that sites $w$ in the highest level are most representative of the behavior of any site on a regular lattice.

In conclusion, we have studied search by a continuous-time quantum walk on fractal networks and, by reference to properties of spectral $\zeta$-functions [14], identified the dominant role of the spectral dimension $d_s$ in controlling the search efficiency and in setting the condition for attaining the Grover limit, for $d_s > 4$. Particularly, we reproduce the known results in regular lattices with integer $d = d_s$ and generalize them to hyper-cubic lattices in arbitrary dimensions $d$ using the Migdal-Kadanoff renormalization group. Although this family of fractals is chosen to satisfy $d_s = d_f = d$, the analysis in Ref. [14] that leads to Eq. (10) implies the preeminence of $d_s$ also for search on other fractals, as had been suggested previously in numerical studies [10].

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