Quantum search in structured database using local adiabatic evolution and spectral methods

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Abstract Since Grover’s seminal work which provides a way to speed up combinatorial search, quantum search has been studied in great detail. We propose a new method for designing quantum search algorithms for finding a marked element in the state space of a graph. The algorithm is based on a local adiabatic evolution of the Hamiltonian associated with the graph. The main new idea is to apply some techniques such as Krylov subspace projection methods, Lanczos algorithm and spectral distribution methods. Indeed, using these techniques together with the second-order perturbation theory, we give a systematic method for calculating the approximate search time at which the marked state can be reached. That is, for any undirected regular connected graph which is considered as the state space of the database, the introduced algorithm provides a systematic and programmable way for evaluation of the search time, in terms of the corresponding graph polynomials.

Keywords Quantum search algorithm · Local adiabatic evolution · Graph · Krylov subspace · Lanczos algorithm · Spectral distribution · Second-order perturbation theory

1 Introduction

Grover’s quantum search algorithm [1] is one of the main applications of quantum computation. This algorithm is sometimes described as a way for searching a marked
item in an unstructured database of $N$ items in time $O(\sqrt{N})$. This gives a quadratic speedup over the exhaustive search for a variety of search problems [2]. But the algorithm as originally proposed is not designed to search a physical database. In [3], Aaronson and Ambainis present a model of query complexity on graphs, where they showed that a database of $N$ items laid out in $d$ spatial dimensions can be searched in time of order $\sqrt{N}$. In [4], Childs and Goldstone have considered an alternative quantum search algorithm based on a continuous time quantum walk on a graph. Quantum walks provide a natural framework for the spatial search problem because the graph can be used to model the locality of the database. In fact, for the case of the complete graph (unsorted database), the resulting algorithm is simply the continuous time search algorithm of Farhi and Gutmann [5]. On the hypercube, their results showed that the algorithm also provides quadratic speedup [6–8]. In [6], Farhi et al. have used the time-dependant Hamiltonian approach for Grover’s problem, where they have considered the constant-rate adiabatic approach (the requirement of adiabaticity is expressed globally) and obtained a complexity of order $N$, the number of items in database. Then, Roland and Cerf [9] have been considered the same problem with the same approach with this deference that they considered the adiabatic evolution locally, i.e., they adjusted the evolution rate of the Hamiltonian so as to keep the evolution adiabatic on each infinitesimal time interval and by this adjusting the total running time of order $\sqrt{N}$ has obtained. Recently, another adiabatic version of the quantum search problem has considered by Rezakhani et al. [10], where they have employed continuous time, global adiabatic evolution in order to calculate a quantity called “adiabatic error”, which quantifies the distance between the instantaneous ground state and the actual marked state.

In this paper, we follow the approach of the paper [9] and employ some techniques such as Krylov subspace projection methods, Lanczos algorithm, spectral distribution methods and the second-order perturbation theory in order to give a systematic method for calculating the total search time approximately. In fact, by reducing the Hilbert space of the corresponding Hamiltonian to the smaller one called Krylov subspace and using the spectral methods, we calculate the minimum energy gap between two lowest eigenvalues of the Hamiltonian and consequently the total search time, in terms of the polynomials associated with the graph. The organization of the paper is as follows: In Sect. 2, we recall some preliminary facts about Krylov subspace projection methods and spectral distribution method needed for the approach of the paper. In Sect. 3, by using the local adiabatic evolution approach, quantum search on a graph is investigated, where an analytical but approximate formula for the quantum search time (the main result of the paper) is obtained in terms of the graph polynomials. Section 4 is devoted to some examples of graphs, in order to clarify the introduced method in details. The last section contains a brief conclusion.

2 Krylov subspace and spectral methods

In this section we give a brief review of some of the main features of Krylov subspace projection methods and spectral distribution method (the reader is referred to Refs. [11–19] for more details).
2.1 Krylov subspace projection methods

Krylov subspace projection methods (KSPM) are probably the most important class of projection methods for linear systems and for eigenvalue problems. In KSPM, approximations to the desired eigenpairs of an \( n \times n \) matrix \( A \) are extracted from a \( d \)-dimensional Krylov subspace

\[
K_d(\langle \phi_0 \rangle, A) = \text{span}\{\langle \phi_0 \rangle, A\langle \phi_0 \rangle, \ldots, A^{d-1}\langle \phi_0 \rangle\},
\]

(2.1)

where \( \langle \phi_0 \rangle \) is often a randomly chosen starting vector called reference state and \( d \ll n \).

In practice, the retrieval of desired spectral information is accomplished by constructing an orthonormal basis \( V_d \in \mathbb{R}^{n \times d} \) of \( K_d(\langle \phi_0 \rangle, A) \) and computing eigenvalues and eigenvectors of the \( d \) by \( d \) projected matrix \( H_d = P_{V_d}^T A P_{V_d} \), where \( P_{V_d} \) is projection operator to \( d \)-dimensional subspace spanned by the basis \( V_d \).

The most popular algorithm for finding an orthonormal basis for the Krylov subspace, is Lanczos algorithm. The Lanczos algorithm transforms a Hermitian matrix \( A \) into a tridiagonal form iteratively, i.e., the matrix \( A \) will be of tridiagonal form in the \( d \)-dimensional projected subspace \( H_d \). In fact, the Lanczos algorithm is deeply rooted in the theory of orthogonal polynomials, which builds an orthonormal sequence of vectors \( \{\langle \phi_0 \rangle, \langle \phi_1 \rangle, \ldots, \langle \phi_{d-1} \rangle\} \) and satisfy the following three-term recursion relations

\[
A\langle \phi_i \rangle = \beta_{i+1}\langle \phi_{i+1} \rangle + \alpha_i\langle \phi_i \rangle + \beta_i\langle \phi_{i-1} \rangle.
\]

(2.2)

The vectors \( \langle \phi_i \rangle, i = 0, 1, \ldots, d - 1 \) form an orthonormal basis for the Krylov subspace \( K_d(\langle \phi_0 \rangle, A) \). In these basis, the matrix \( A \) is projected to the following symmetric tridiagonal matrix:

\[
A = \begin{pmatrix}
\alpha_0 & \beta_1 & 0 & \cdots & \cdots \\
\beta_1 & \alpha_1 & \beta_2 & 0 & \cdots \\
0 & \beta_2 & \alpha_2 & \beta_3 & \cdots \\
\vdots & \vdots & \ddots & \ddots & \ddots \\
\cdots & 0 & \beta_{d-2} & \alpha_{d-2} & \beta_{d-1} \\
\cdots & \cdots & \cdots & 0 & \beta_{d-1} & \alpha_{d-1}
\end{pmatrix},
\]

(2.3)

where the scalars \( \beta_{i+1} \) and \( \alpha_i \) are computed to satisfy two requirements, namely that \( \langle \phi_{i+1} \rangle \) be orthogonal to \( \langle \phi_i \rangle \) and that \( \|\langle \phi_{i+1} \rangle\| = 1 \).

In fact, the Lanczos algorithm is a modified version of the classical Gram-Schmidt orthogonalization process. As it can be seen, at its heart is an efficient three-term recursion relation which arises because the matrix \( A \) is real and symmetric.

If we define the Krylov matrix \( K \) such that the columns of \( K \) are Krylov basis \( \{A^i\phi_0; i = 0, \ldots, d - 1\} \) as:

\[
K := (\langle \phi_0 \rangle, A\langle \phi_0 \rangle, \ldots, A^{d-1}\langle \phi_0 \rangle),
\]

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the application of the orthonormalization process to the Krylov matrix is equivalent to the construction of an upper triangular matrix $P$ such that the resulting sequence $\Phi = KP$ satisfies $\Phi^\dagger \Phi = 1$. We denote by $|\phi_i\rangle$ and $P_j$ respectively the $j$-th column of $\Phi$ and $P$. Then we have

$$\langle \phi_0|P_i^\dagger (A)P_j(A)|\phi_0\rangle = \langle KP_i|KP_j\rangle = \langle \phi_i|\phi_j\rangle,$$  

(2.4)

where $P_i = a_0 + a_1 A + \cdots + a_i A^i$ is a polynomial of degree $i$ in indeterminate $A$.

In the remaining part of this section we give an algorithmic outline of the Lanczos algorithm, where it will be used in calculation of parameters $\alpha_i$ and $\beta_i$ appeared in (2.2).

**Lanczos algorithm**

Input: Matrix $A \in \mathbb{R}^{n \times n}$, starting vector $|\phi_0\rangle$, $||\phi_0|| = 1$, scalar $d$

Output: Orthogonal basis $\{ |\phi_0\rangle, \ldots, |\phi_{d-1}\rangle \}$ of Krylov subspace $K_d(|\phi_0\rangle, A)$

$$\begin{align*}
\beta_0 &= 0, |\phi_0\rangle = |\phi\rangle/||\phi|| \quad \text{for} \quad i = 0, 1, 2, \\
|\upsilon_i\rangle &= A|\phi_i\rangle \\
\alpha_i &= \langle \phi_i|\upsilon_i\rangle \\
|\upsilon_{i+1}\rangle &= |\upsilon_i\rangle - \beta_i|\phi_{i-1}\rangle - \alpha_i|\phi_i\rangle \\
\beta_{i+1} &= |||\upsilon_{i+1}\rangle|| \quad \text{if} \quad \beta_{i+1} \neq 0 \\
|\phi_{i+1}\rangle &= |\upsilon_{i+1}\rangle/\beta_{i+1} \quad \text{else} \quad |\phi_{i+1}\rangle = 0.
\end{align*}$$

2.2 Spectral distribution method

For any pair $(A, |\phi_0\rangle)$ of a matrix $A$ and a vector $|\phi_0\rangle$, one can assign a measure $\mu$ as follows

$$\mu(x) = \langle \phi_0|E(x)|\phi_0\rangle,$$  

(2.5)

where $E(x) = \sum_i |u_i\rangle\langle u_i|$ is the operator of projection onto the eigenspace of $A$ corresponding to eigenvalue $x$, i.e.,

$$A = \int x E(x)dx$$  

(2.6)

so that, for any polynomial $P(A)$ we have

$$P(A) = \int P(x)E(x)dx,$$  

(2.7)

where for discrete spectrum the above integrals are replaced by summation. For example, in continuous time quantum walk on a graph [22,23], the expectation value of
powers of the corresponding adjacency matrix $A$ over starting site $|\phi_0\rangle$ can be written as

$$\langle \phi_0 | A^m | \phi_0 \rangle = \int_R x^m \mu(dx), \quad m = 0, 1, 2, \ldots$$  \hspace{1cm} (2.8)

The existence of a spectral distribution satisfying (2.8) is a consequence of Hamburgers theorem, see e.g., Shohat and Tamarkin ([16], Theorem 1.2).

From the orthogonality of vectors $|\phi_j\rangle$ (Krylov bases) produced from Lanczos algorithm process we have,

$$\delta_{ij} = \langle \phi_i | \phi_j \rangle = \langle \phi_0 | P_i^\dagger (A) P_j (A) | \phi_0 \rangle \nonumber = \int P_i^*(x) P_j(x) \mu(x) dx = (P_i, P_j)_\mu. \hspace{1cm} (2.9)$$

Conversely if $P_0, \ldots, P_{d-1}$ is the system of orthonormal polynomials for the measure $\mu$ then the vectors

$$|\phi_j\rangle = P_j (A) |\phi_0\rangle, \hspace{1cm} (2.10)$$

will coincide with the sequence of orthonormal vectors produced by the Lanczos algorithm applied to $(A, |\phi_0\rangle)$.

Now, substituting (2.10) in (2.2), we get three term recursion relations between polynomials $P_j (A)$, which leads to the following three term recursion between polynomials $P_j(x)$

$$\beta_{k+1} P_{k+1}(x) = (x - \alpha_k) P_k(x) - \beta_k P_{k-1}(x) \hspace{1cm} (2.11)$$

for $k = 0, \ldots, d - 1$. Multiplying by $\beta_1 \ldots \beta_k$ we obtain

$$\beta_1 \ldots \beta_{k+1} P_{k+1}(x) = (x - \alpha_k) \beta_1 \ldots \beta_k P_k(x) - \beta_k^2 \beta_1 \ldots \beta_{k-1} P_{k-1}(x). \hspace{1cm} (2.12)$$

By rescaling $P_k$ as $Q_k = \beta_1 \ldots \beta_k P_k$, the three term recursion relations (2.11) are replaced by

$$Q_0(x) = 1, \quad Q_1(x) = x, \quad Q_{k+1}(x) = (x - \alpha_k) Q_k(x) - \beta_k^2 Q_{k-1}(x), \hspace{1cm} (2.13)$$

for $k = 1, 2, \ldots, d$.

In the next section, we will need the distinct eigenvalues of adjacency matrix of a given undirected graph which can be written in the form (2.3), and the corresponding eigenvectors in order to obtain the minimum time at which the marked state can be reached. As it is known from spectral theory, we have the eigenvalues $x_i$ of the adjacency matrix $A$ as roots of the last polynomial $Q_{d+1}(x)$ in (2.13), and the normalized eigenvectors as [18, 19]
$|\psi_i\rangle = \frac{1}{\sqrt{\sum_{l=0}^{d} P_l^2(x_i)}} \begin{pmatrix} P_0(x_i) \\ P_1(x_i) \\ \vdots \\ P_d(x_i) \end{pmatrix}$. (2.14)

3 Quantum search via local adiabatic evolution

In this section, we investigate quantum search in an structured database by using the time-dependent Hamiltonian approach and spectral distribution method. To do so, first, we recall briefly the time-dependent Hamiltonian approach, adiabatic theorem and the local adiabatic evolution employed in Ref. [9] to Grover’s problem.

3.1 The quantum adiabatic theorem

The quantum adiabatic theorem refers to a situation in which the original Hamiltonian of a system is gradually changed into a new Hamiltonian. Roughly speaking, the theorem states that, if the change in the Hamiltonian occurs sufficiently slowly, the dynamics remain relatively simple, in the sense that, if the system begins close to an eigenstate, it remains approximately close to an eigenstate.

More generally, for $s \in [0, 1]$, let $H(s)$ be a Hermitian operator that varies smoothly as a function of $s$. Let $s := t/T$. Then for $T$ arbitrarily large, $H(t)$ varies arbitrarily slowly as a function of $t$. Consider the evolution of a quantum system state $|\psi(t)\rangle$ subject to $H(t)$ is described by the Schrödinger equation ($\hbar = 1$)

$$i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle. \quad (3.1)$$

Now suppose that $|\psi(0)\rangle$ is an eigenstate of $H(0)$, which can be assumed for simplicity as the ground state, and is nondegenerate. Furthermore, suppose that the ground state of $H(s)$ is nondegenerate for all values of $s \in [0, 1]$. Then the adiabatic theorem says that in the limit $T \to \infty$, the final evolved state $|\psi(T)\rangle$, will be the ground state of $H(1)$. Of course, evolution for an infinite time is rather impractical. For computational purposes, we need a quantitative version of the adiabatic theorem: we would like to understand how large $T$ must be so that the final state is guaranteed to differ from the adiabatically evolved state by at most some fixed small amount. In particular, we would like to understand how the required evolution time depends on spectral properties of the interpolating Hamiltonian $H(s)$. In fact, as it will be seen, the timescale for adiabaticity is intimately connected to the energy gap between the ground and first excited states.

More clearly, according to the adiabatic theorem [20,21], the state of the system will stay close to the instantaneous ground state of the Hamiltonian at each time $t$, if the Hamiltonian varies slowly enough. In other words, for the instantaneous energy eigenbasis defined by $H(t) |E_n(t)\rangle = E_n(t) |E_n(t)\rangle$, if we define the minimum gap between the lowest two eigenvalues as
\[ g_{\text{min}} = \min_{0 \leq t \leq T} [E_1(t) - E_0(t)] \]  

(3.2)

and the maximum value of the matrix element of \( \frac{dH}{dt} \) between the two corresponding eigenstates as

\[ D_{\text{max}} = \max_{0 \leq t \leq T} |\langle \frac{dH}{dt} \rangle_{1,0}| \]  

(3.3)

with \( (\frac{dH}{dt})_{1,0} = \langle E_1(t) | \frac{dH}{dt} | E_0(t) \rangle \), then the adiabatic evolution theorem guarantees that for the system which is prepared in its ground state \( |E_0(0)\rangle \) at time \( t = 0 \), and evolved under the Hamiltonian \( H(t) \), we will have

\[ |\langle E_0(T) | \psi(T) \rangle|^2 \geq 1 - \epsilon^2 \]  

(3.4)

provided that

\[ \frac{D_{\text{max}}}{g_{\text{min}}}^2 \leq \epsilon, \]  

(3.5)

where \( \epsilon \ll 1 \).

3.2 Quantum search in an unsorted database with local adiabatic evolution

Assuming a set of \( N \) items in an unsorted database (uniform distribution) where one of them is marked, the main goal is finding the marked item in a minimum run time. To this end, a quantum state \( |i\rangle \) is assigned to each item \( i \), so that the state space of the database is spanned by the states \( |i\rangle \) with \( i = 0, 1, \ldots, N-1 \), where the marked state is denoted by \( |m\rangle \). Since \( |m\rangle \) is unknown a priori, the initial state is chosen as an equal superposition of all basis states, i.e.,

\[ |\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle. \]  

(3.6)

Then, the Hamiltonian of the system is initially chosen as

\[ H_0 = I_N - |\psi_0\rangle \langle \psi_0| \]  

(3.7)

whose ground state is \( |\psi_0\rangle \) with energy zero. Since the database is unsorted, we can associate the items of the database with the nodes of the complete graph with \( N \) vertices (denoted by \( K_N \)), for which the adjacency matrix is given by \( A = J_N - I_N \). Therefore the initial Hamiltonian can be written as
\[ H_0 = I_N - \frac{1}{N} \sum_{i,j=0}^{N-1} |i\rangle \langle j| = I_N - \frac{1}{N} J_N = \frac{1}{N} [(N - 1)I_N - A] = \frac{1}{N} L, \quad (3.8) \]

where, \( J_N \) is an \( N \times N \) all one matrix and \( L = (N - 1)I_N - A \) is the Laplacian of the complete graph \( K_N \). Now, suppose that we are able to apply to our system the Hamiltonian

\[ H_m = I_N - |m\rangle \langle m|, \quad (3.9) \]

whose ground state is the unknown marked state \(|m\rangle\). Then, the corresponding time dependent Hamiltonian is considered as the following linear interpolation between \( H_0 \) and \( H_m \)

\[ H(s) = (1-s)H_0 + s H_m = \frac{1}{N} [(N - 1 + s)I_N - (1-s)A - Ns|m\rangle \langle m|], \quad (3.10) \]

where \( s \) is an evolution function of time \( t \) and must be found optimally with the boundary conditions \( s(0) = 0 \) and \( s(T) = 1 \). As discussed in the previous subsection, in the global adiabatic evolution \( s(t) \) is chosen as a linear function of \( t \) as \( s(t) = t/T \), but in the local adiabatic evolution the time interval \( T \) is divided into infinitesimal time intervals \( dt \) and the adiabaticity condition is locally applied to each of these intervals. Applying Eq. (3.5) to each infinitesimal time intervals, the local adiabatic condition is given by

\[ |\frac{ds}{dt}| \leq \frac{\epsilon}{g^2(s)} |\langle \frac{dH}{dt} \rangle_{1.0}| \]  

(3.11)

for all times \( t \). Now, by using the fact that \( |\langle \frac{dH}{dt} \rangle_{1.0}| \leq 1 \), the condition (3.11) is verified provided that

\[ |\frac{ds}{dt}| = \epsilon g^2(s). \quad (3.12) \]

The algorithm consists in preparing the system in the state \(|\psi_0\rangle\) and then applying the Hamiltonian \( H(s) \) during a time \( T \) so that \( s(T) = 1 \). In order to obtain the eigenvalues of \( H(s) \) and evaluate (3.2), we use the Lanczos algorithm to obtain the orthonormal basis in which the hamiltonian \( H(s) \) can be reduced to as a tridiagonal matrix. To do so, we choose \(|m\rangle \equiv |\phi_0\rangle\) as the reference state (starting vector in the Lanczos iteration algorithm) and apply \( H(s) \) on it to obtain the vector orthogonal to \(|\phi_0\rangle\) as

\[ |\phi_1\rangle = \frac{1}{\sqrt{N-1}} \left( \sqrt{N} |\psi_0\rangle - |\phi_0\rangle \right). \]
Now, the Hamiltonian $H(s)$ can be represented in the new orthonormal basis states $|\phi_0\rangle$ and $|\phi_1\rangle$ as follows

$$H(s) = \frac{1}{N} \begin{pmatrix} (1 - s)(N - 1) & -\sqrt{N - 1}(1 - s) \\ -\sqrt{N - 1}(1 - s) & 1 + s(N - 1) \end{pmatrix}$$

(3.13)

The eigenvalues of $H(s)$ are given by $E_\pm = \frac{1}{2N} \left\{ N \pm \sqrt{N^2(1 - 2s)^2 + 4Ns(1 - s)} \right\}$, so that the difference between these two eigenvalues gives the gap $g(s)$ as

$$g(s) = \sqrt{\frac{N - 4s(1 - s)(N - 1)}{N}}.$$  

(3.14)

We see that the minimum gap $g_{\text{min}} = \frac{1}{\sqrt{N}}$ is attained for $s = 1/2$. Now, by using the local adiabatic condition (3.12) we obtain

$$\left| \frac{ds}{dt} \right| = \frac{\epsilon}{N} [N - 4s(1 - s)(N - 1)].$$

(3.15)

After integration, one can find

$$t = \frac{1}{2\epsilon} \frac{N}{\sqrt{N - 1}} \left\{ \arctan[\sqrt{N - 1}(2s - 1)] + \arctan \sqrt{N - 1} \right\}.$$  

(3.16)

One may now evaluate the computation time of the algorithm by taking $s = 1$. For $N \gg 1$, we obtain

$$T \simeq \frac{\pi}{2\epsilon} \sqrt{N},$$

(3.17)

which gives a quadratic speed-up with respect to a classical search, so that the algorithm can be viewed as the adiabatic evolution version of Grover’s algorithm.

3.3 Quantum search in a structured (non-uniform) database

In the case that our states distributed non-uniformly, the state space of the database can be considered as an arbitrary connected graph other than the complete graph. Therefore, a straightforward generalization of the relations (3.8)–(3.10) leads us to consider

$$H_0 = \gamma L, \quad H_m = I - |m\rangle\langle m|$$

(3.18)

so that

$$\tilde{H}(s) = \gamma (1 - s)L + s(I - |m\rangle\langle m|) = aI_N - \gamma (1 - s)A - s|m\rangle\langle m|,$$

(3.19)
where $L$ is the Laplacian of the graph and $\gamma$ is a constant parameter which is determined in such a way that the search time be minimum (the search algorithm be optimal). We will consider regular undirected graphs so that the corresponding adjacency matrices are symmetric, and moreover the Laplacian $L$ and the adjacency matrix $A$ of the graphs differ from each other in only multiple of identity matrix, i.e., we have $L = DI - A$ with $D$ as the degree of each vertex. So, the parameter $a$ in (3.19) is given by $a = \gamma D(1-s) + s$. Since we need the minimum gap between two lowest eigenvalues of the hamiltonian $\tilde{H}(s)$, so the first term in (3.19) (multiple of identity) can be dropped.

By choosing $|m\rangle \equiv |\phi_0\rangle$ as the starting state for the Lanczos iteration algorithm, the corresponding Krylov bases are obtained via the three term recursion relation (2.2). That is we have,

$$
\tilde{H}(s)|\phi_i\rangle = \gamma(s-1)\alpha_0|\phi_i\rangle + \gamma(s-1)\beta_1|\phi_1\rangle,
$$

$$
\tilde{H}(s)|\phi_i\rangle = \gamma(s-1)(\beta_i|\phi_{i-1}\rangle + \alpha_i|\phi_i\rangle + \beta_{i+1}|\phi_{i+1}\rangle) ; \quad i = 1, 2, \ldots, d. \quad (3.20)
$$

In other words, in the krylov bases $|\phi_i\rangle$, the Hamiltonian $\tilde{H}(s)$ is rewritten as

$$
\tilde{H}(s) = \gamma(s-1)H_0 - sH_1
$$

where,

$$
H_0 \equiv A = \begin{pmatrix}
\alpha_0 & \beta_1 & 0 & 0 & \cdots & 0 \\
\beta_1 & \alpha_1 & \beta_2 & 0 & \cdots & 0 \\
0 & \beta_2 & \alpha_2 & \beta_3 & \cdots & 0 \\
0 & 0 & \beta_3 & \alpha_3 & \beta_4 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\
0 & 0 & \cdots & 0 & \beta_{d-1} & \alpha_{d-1}
\end{pmatrix}, \quad H_1 = \begin{pmatrix}
1 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 \\
\vdots & 0 & \ddots & \ddots \\
0 & 0 & \cdots & 0
\end{pmatrix}. \quad (3.22)
$$

Now, using (2.14) and the form of $H_1$, one can easily evaluate

$$
\langle \psi_j | H_1 | \psi_i \rangle = \frac{1}{\sqrt{\sum_{i,j'=0}^{d} P_i^2(x_j) P_i^2(x_i)}},
$$

so that we obtain

$$
E_i^{(1)} = \langle \psi_i | H_1 | \psi_i \rangle = \frac{1}{\sum_{i=0}^{d} P_i^2(x_i)},
$$

$$
E_i^{(2)} = \sum_{j:j \neq i} \frac{|\langle \psi_j | H_1 | \psi_i \rangle|^2}{E_i^{(0)} - E_j^{(0)}} = \frac{1}{\gamma(s-1)} \sum_{j:j \neq i} \frac{1}{(x_i - x_j) \sum_{i,j'=0}^{d} P_i^2(x_i) P_i^2(x_j)}. \quad (3.22)
$$

Then, the approximate eigenvalues of $\tilde{H}(s)$ up to second order are given by

$$
E_i \simeq \gamma(s-1)x_i - sE_i^{(1)} + s^2 E_i^{(2)},
$$

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such that, the energy gap $g(s)$ is given by

$$g(s) = E_1 - E_0 \cong \gamma(s - 1)(x_1 - x_0) - s \left( \frac{1}{\sum_{l=0}^{d} P_l^2(x_1)} - \frac{1}{\sum_{l=0}^{d} P_l^2(x_0)} \right)$$

$$+ \frac{s^2}{\gamma(s - 1)} \left\{ \sum_{j \neq 1} \frac{1}{(x_1 - x_j)} \sum_{l,l'=0}^{d} P_l^2(x_1) P_{l'}^2(x_j) \right\} - \sum_{j \neq 0} \frac{1}{(x_0 - x_j)} \sum_{l,l'=0}^{d} P_l^2(x_0) P_{l'}^2(x_j) \}.$$  \hspace{1cm} (3.23)

Denoting the terms in the parentheses of the second term in (3.23) by $A$ and the terms in the bracket of the last term by $B$, the energy gap is written as:

$$g(s) \cong \gamma(s - 1)(x_1 - x_0) - sA + \frac{s^2}{\gamma(s - 1)}B.$$  \hspace{1cm} (3.24)

Now, in order to obtain the critical value of $\gamma$ in which the gap $g(s)$ is minimum, we take the derivative of $g(s)$ with respect to $\gamma$ so that $\frac{dg(s)}{d\gamma} = 0$. Then, one can obtain $\gamma_{\text{crit.}} = \frac{s}{1 - s} \sqrt{\frac{B}{(x_1 - x_0)}}, \ s \neq 0, 1$. \hspace{1cm} (3.25)

By substituting $\gamma_{\text{crit.}}$ in (3.24), we obtain

$$g_{\text{min}}(s) \cong -s \left[ A + 2\sqrt{B(x_1 - x_0)} \right].$$  \hspace{1cm} (3.26)

Now, by using (3.12), the search time is evaluated as

$$t \cong \int \frac{ds}{\epsilon s^2(A + 2\sqrt{B(x_1 - x_0)})^2} = \frac{1}{\epsilon s (A + 2\sqrt{B(x_1 - x_0)})^2}.$$  

By substituting $s = 1$, the total search time at which the marked state $|m\rangle$ is found, is given by

$$T \cong \frac{1}{\epsilon (A + 2\sqrt{B(x_1 - x_0)})^2}.$$  \hspace{1cm} (3.27)

As the above result indicates, in order to obtain the search time, one needs to evaluate the terms $A$ and $B$ defined below of (3.23) in terms of the corresponding graph polynomials $P_l(x)$. On the other hand, $A$ and $B$ can be calculated easily via a systematic computer program for calculating the corresponding polynomials from the three term recursion relations (2.11).
4 Examples

4.1 Cyclic graph $C_n$

A well known example of regular graphs, is the cyclic graph with $N$ vertices denoted by $C_N$. We consider the cyclic graph with even number of vertices, $N = 2m$, the case of odd $N$ can be considered similarly. For even number of vertices $N = 2m$, the adjacency matrices are given by

$$A_0 = I_{2m}, \quad A_i = S^i + S^{-i}, \quad i = 1, 2, \ldots, m - 1, \quad A_m = S^m,$$

(4.1)

where, $S$ is the $N \times N$ Shift matrix with period $N$, i.e., $S^N = I_N$, defined as follows

$$S = \begin{pmatrix}
0 & 1 & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & 1 & 0 \\
0 & 0 & \cdots & 0 & 1 \\
1 & 0 & \cdots & 0 & 0
\end{pmatrix},$$

(4.2)

so that, we have $S|i\rangle = |i + N - 1\rangle$ for $i = 0, 1, \ldots, N - 1$. For the graph $C_{2m}$ we assign $m + 1$ strata $|\phi_i\rangle$ given by

$$|\phi_0\rangle = |0\rangle, \quad |\phi_i\rangle = \frac{1}{\sqrt{2}}(|i\rangle + |N - i\rangle), \quad i = 1, \ldots, m - 1; \quad |\phi_m\rangle = |m\rangle.$$

Then, by using (4.1), one can obtain the following relations

$$A_1|\phi_0\rangle = \sqrt{2}|\phi_1\rangle, \quad A_1|\phi_i\rangle = |\phi_{i+1}\rangle + |\phi_{i-1}\rangle, \quad i = 2, \ldots, m - 2; \quad A_1|\phi_{m-1}\rangle = |\phi_{m-2}\rangle + \sqrt{2}|\phi_m\rangle, \quad A_1|\phi_m\rangle = \sqrt{2}|\phi_{m-1}\rangle.$$

(4.3)

By comparing (4.3) with three term recursion relations (2.2), we obtain the corresponding QD parameters as

$$\alpha_i = 0, \quad i = 0, 1, \ldots, m; \quad \beta_1 = \beta_m = \sqrt{2}; \quad \beta_i = 1, \quad i = 2, \ldots, m - 1.$$

(4.4)

Then by using the three term recursion relations (2.13), and using $P_k(x) = \frac{1}{\beta_1 \cdots \beta_k} Q_k(x)$, the corresponding polynomials $P_i(x)$ are calculated as

$$P_0(x) = 1, \quad P_i(x) = \sqrt{2}T_i \left( \frac{x}{2} \right), \quad i = 1, \ldots, m - 1; \quad P_m(x) = T_m \left( \frac{x}{2} \right),$$

where, $T_i(x)$ are the Tchebichef polynomials of the first kind. Therefore, $x_i$’s are the roots of $T_{m+1}(\frac{x}{2})$ which are given as

$$x_i = 2 \cos \left( \frac{\pi i}{m} \right), \quad i = 0, 1, \ldots, m,$$
particularly, we have \( x_0 = 2 \) and \( x_1 = 2 \cos \frac{\pi}{m} \) such that \( x_1 - x_0 = 2(1 - \cos \frac{\pi}{m}) \). Now, in order to calculate the minimum energy gap \( g_{\text{min}} \), and the corresponding search time \( T \), we need to calculate \( A \) and \( B \) appearing in (3.26) and (3.27). By substituting the above \( P_t(x) \), we need to calculate the following quantities

\[
A = \frac{1}{1 + T_m^2(\cos \frac{\pi}{m}) + 2 \sum_{i=1}^{m-1} T_i^2(\cos \frac{\pi}{m})} = \frac{1}{1 + T_m^2(1) + 2 \sum_{i=1}^{m-1} T_i^2(1)}
\]

and

\[
B = \frac{1}{4m} \left\{ \sum_{j \neq 1} \left( \cos \frac{\pi}{m} - \cos \frac{\pi j}{m} \right) \sum_{l=0}^{m-1} T_l^2(\cos \frac{\pi j}{m}) \right. \\
- \sum_{j \neq 0} 2 \left( 1 - \cos \frac{\pi j}{m} \right) \sum_{l=0}^{m-1} T_l^2(\cos \frac{\pi j}{m}) \right\}.
\]

By using \( T_l(x) = \cos(l \cos^{-1} x) \), we have \( T_l(\frac{x}{2}) = T_l(\cos(\frac{x}{2} \cos^{-1} x)) = \cos(l \cos^{-1} (\cos(\frac{\pi j}{m}))) = \cos(\frac{\pi l j}{m}) \), for \( j, l = 0, 1, \ldots, m \). In particular, we have \( T_l(x_1/2) = \cos(\frac{\pi l j}{m}) \), \( T_l(x_0/2) = 1 \), so that we obtain

\[
A = \frac{1}{2} \left\{ \frac{1}{\sum_{i=0}^{m-1} \cos^2(\frac{\pi i}{m})} - \frac{1}{m} \right\} = \frac{1}{2} \left( \frac{2}{m} - \frac{1}{m} \right) = \frac{1}{2m},
\]

where, in the second equality we have used the following calculation

\[
\sum_{k=0}^{m-1} \cos^2 \left( \frac{\pi k}{m} \right) = \sum_{k=0}^{m-1} \frac{1 + \cos \left( \frac{2\pi k}{m} \right)}{2} = \frac{1}{2} \left( m + \sum_{k=0}^{m-1} \cos \left( \frac{2\pi k}{m} \right) \right) \\
= \frac{1}{2} \left( m + \frac{1}{2} \sum_{k=0}^{m-1} (\omega^k + \omega^{-k}) \right) = \frac{m}{2}
\]

with \( \omega := e^{\frac{2\pi i}{m}} \) so that \( \sum_{k=0}^{m-1} \omega^k = \sum_{k=0}^{m-1} \omega^{-k} = 0 \). The quantity \( B \) is calculated similarly, as

\[
B = \frac{1}{4m^2} \left\{ \sum_{j \neq 1} \left( \frac{2}{\cos \frac{\pi}{m} - \cos \frac{\pi j}{m}} (1 + \delta_{j,0}) \right) - \sum_{j \neq 0} \frac{1}{1 - \cos \frac{\pi j}{m}} \right\},
\]

where, we have used

\[
\sum_{l=0}^{m-1} T_l^2 \left( \cos \frac{\pi j}{m} \right) = \sum_{l=0}^{m-1} \cos^2 \left( \frac{\pi l j}{m} \right) = \frac{m}{2} + \frac{1}{4} \sum_{l=0}^{m-1} (\omega^{lj} + \omega^{-lj}) = \frac{m}{2} (1 + \delta_{j,0}) .
\]
Now, one can easily evaluate

\[ B(x_1 - x_0) = \frac{1}{m^2} \left\{ 1 + \frac{\cos \left( \frac{\pi}{m} \right) - 1}{2} \sum_{j \neq 0,1} \frac{2 - \left( \cos \left( \frac{\pi}{m} \right) + \cos \left( \frac{\pi j}{m} \right) \right)}{\left( \cos \left( \frac{\pi}{m} \right) - \cos \left( \frac{\pi j}{m} \right) \right) \left( 1 - \cos \left( \frac{\pi j}{m} \right) \right)} \right\}. \]

Finally, by replacing in (3.26) and (3.27) respectively, we obtain the corresponding minimum gap and the total search time as

\[ \text{g}_{\text{min}}(s) \approx -\frac{s}{2m} \left\{ 1 + 4 \left[ 1 + \frac{\cos \left( \frac{\pi}{m} \right) - 1}{2} \sum_{j \neq 0,1} \frac{2 - \left( \cos \left( \frac{\pi}{m} \right) + \cos \left( \frac{\pi j}{m} \right) \right)}{\left( \cos \left( \frac{\pi}{m} \right) - \cos \left( \frac{\pi j}{m} \right) \right) \left( 1 - \cos \left( \frac{\pi j}{m} \right) \right)} \right] \right\}^{1/2}, \]

and

\[ T \approx \frac{4m^2}{\varepsilon} \left\{ 1 + 4 \left[ 1 + \frac{\cos \left( \frac{\pi}{m} \right) - 1}{2} \sum_{j \neq 0,1} \frac{2 - \left( \cos \left( \frac{\pi}{m} \right) + \cos \left( \frac{\pi j}{m} \right) \right)}{\left( \cos \left( \frac{\pi}{m} \right) - \cos \left( \frac{\pi j}{m} \right) \right) \left( 1 - \cos \left( \frac{\pi j}{m} \right) \right)} \right] \right\}^{1/2}, \]

respectively. It can be seen that in the limit of large \( m \), where \( \cos \left( \frac{\pi}{m} \right) \rightarrow 1 \), the minimum gap and the total search time, respectively tend to the following values

\[ \text{g}_{\text{min}}(s) \approx -\frac{s}{2m}, \]

\[ T \approx \frac{4m^2}{25\varepsilon}. \]

4.2 Dihedral group graph

The dihedral group \( G = D_{2n} \) is generated by two generators \( a \) and \( b \) as follows:

\[ D_{2n} = \langle a, b : a^n = 1, b^2 = 1, b^{-1}ab = a^{-1} \rangle. \]

We consider the even \( n = 2m \), where the odd \( n \) can be considered similarly. In this case, the conjugacy classes of the group, are given by

\[ C_0 = \{e\}, \quad C_i = \{a^i, a^{-i}\}; \quad i = 1, \ldots, m - 1, \]

\[ C_m = \{a^m\}, \quad C_{m+1} = \{a^{2j} b; \quad 0 \leq j \leq m - 1\} \quad C_{m+2} = \{a^{2j+1} b; \quad 0 \leq j \leq m - 1\}, \]

so we have \( m + 3 \) conjugacy classes. It is well known that the adjacency matrices defined as \( A_i = \sum_{g \in C_i} R(g) \), are correspond to the underlying graph of the so-called group association scheme \([23–25]\) associated with the group \( D_{2n} \), where \( R(g) \) is the regular representation of the element \( g \) of the group \([26]\). Therefore, we have

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\[ A_0 = I_2 \otimes I_n, \quad A_i = I_2 \otimes (S^i + S^{-i}), \quad i = 1, 2, \ldots, m - 1, \]
\[ A_m = I_2 \otimes S^m, \quad A_{m+1} = \sigma_x \otimes (I_n + S^2 + \cdots + S^{(m-1)}), \]
\[ A_{m+2} = \sigma_x \otimes (S + S^3 + \cdots + S^{2(m-1)}) \]

where, \( S \) is the shift matrix defined in the previous example, and \( \sigma_x \) is the Pauli matrix. In order that we obtain a connected undirected graph, the adjacency matrices must be symmetrized, i.e., \( A_i = A_i^t \). To this end, we introduce the new adjacency matrix \( A' \) as

\[ A' = A_{m+1} + A_{m+2} = \sigma_x \otimes (I + S + \cdots + S^{n-1}) \]

so that the Krylov bases are given by

\[ |\phi_0\rangle = \{|e\rangle\}, \]
\[ |\phi_1\rangle = \frac{1}{\sqrt{n}}(|b\rangle + |ba\rangle + |ba^{n-1}\rangle), \]
\[ |\phi_2\rangle = \frac{1}{\sqrt{n-1}}(|a\rangle + |a^2\rangle + |a^{n-1}\rangle) \]

and the adjacency matrix is represented as

\[
A' = \begin{pmatrix}
0 & \sqrt{n} & 0 \\
\sqrt{n} & 0 & \sqrt{n(n-1)} \\
0 & \sqrt{n(n-1)} & 0
\end{pmatrix}.
\]

By replacing \( \alpha_0 = \alpha_1 = \alpha_2 = 0; \beta_1 = \sqrt{n}, \beta_2 = \sqrt{n(n-1)} \) in the three term recursion relation (2.13), the corresponding polynomials are obtained as

\[ Q_0(x) = 1, \quad Q_1(x) = x, \quad Q_2(x) = x^2 - n, \quad Q_3(x) = x(x^2 - n^2). \]

So, the corresponding eigenvalues are given by \( x_0 = -n, x_1 = 0 \) and \( x_2 = n \) (the roots of \( Q_3(x) \)). Then by replacing in (3.23), (3.26) and (3.27) respectively, and considering \( n \gg 1 \), we obtain

\[ A = \frac{2n - 3}{2n} \approx 1, \quad B = \frac{4n - 3}{4n^3} \approx \frac{1}{2n^2}, \quad \gamma_{\text{crit.}} \approx \frac{s}{1 - s} \frac{\sqrt{4n - 3}}{2n^2}, \]
\[ g_{\text{min}}(s) \approx s \left( \frac{2n + 2 \sqrt{4n - 3} - 3}{2n} \right), \quad T \approx \frac{4n^2}{\varepsilon (2n + 4 \sqrt{n})^2}. \]

4.3 m-Partite graph

An \( m \)-partite graph (i.e., a set of graph vertices decomposed into \( m \) disjoint sets such that no two graph vertices within the same set are adjacent) such that every pair of
graph vertices in the \( m \) sets are adjacent. Considering an \( m \)-partite graph which has \( n \) vertices in each of its disjoint sets, the corresponding adjacency matrix is given by

\[
A = K_m \otimes J_n,
\]

where, \( K_m \) is the adjacency matrix of the complete graph with \( m \) vertices and \( J_n \) is \( n \times n \) all one matrix. Now by using the Lanczos iteration algorithm, the Krylov bases are obtained as

\[
|\phi_0\rangle = |1\rangle, \\
|\phi_1\rangle = \frac{1}{\sqrt{n(m-1)}}(|n + 1) + |n + 2) + \cdots + |n(m - 1))\rangle, \\
|\phi_2\rangle = \frac{1}{\sqrt{(n-1)}}(2) + |3) + \cdots + |n))
\]

where, the adjacency matrix is reduced to the following \( 3 \times 3 \) tridiagonal form

\[
A = \begin{pmatrix}
0 & \frac{\sqrt{n(m-1)}}{n} & 0 \\
\frac{\sqrt{n(m-1)}}{n} & \frac{n-1}{n(m-1)} & \frac{\sqrt{n-1}(m-1)}{(n-1)(m-1)} \\
0 & \frac{\sqrt{n-1}(m-1)}{(n-1)(m-1)} & 0
\end{pmatrix}.
\]

Now, as illustrated in the previous example in detail, by replacing \( \alpha_0 = \alpha_2 = 0, \alpha_1 = n(m-2) \) and \( \beta_1 = \sqrt{n(m-1)}, \beta_2 = \sqrt{n(m-1)(n-1)} \) in three term recursion relations (2.13), and evaluating the polynomials \( P_i(x) \) for \( i = 0, 1, 2 \) and \( Q_3(x) \), one can obtain

\[
x_0 = -n, \quad x_1 = 0, \quad x_2 = n(m-1)
\]

and

\[
A = \frac{m(n-1) - 1}{mn}, \quad B = \frac{1}{n} \left[ \frac{1}{n^2 m(m-1)} \right] + \frac{1}{nm} \left[ \frac{m^2 n - 2m + 1}{n^2 m^2 (m-1)} \right],
\]

where for \( n \gg 1, m \gg 1 \), \( A \) and \( B \) are approximately as

\[
A \approx 1, \quad B \approx \frac{1}{n^2}.
\]

Then, by using (3.25), (3.26) and (3.27), one can obtain

\[
\gamma_{crit.} \approx \frac{s}{1 - s} \sqrt{\frac{1}{n^3(m-1)}}, \\
g_{\min}(s) \approx s \left( 1 + 2 \sqrt{\frac{m-1}{n}} \right).
\]
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\[
T \cong \frac{1}{\varepsilon \left(1 + 2\sqrt{\frac{m-1}{n}}\right)^2},
\]

respectively.

4.4 Crown graph

A crown graph on \(2n\) vertices is an undirected graph with two sets of vertices \(u_i\) and \(v_i\) and with an edge from \(u_i\) to \(v_j\) whenever \(i \neq j\). The adjacency matrix of this graph is given by:

\[
A = K_n \otimes \sigma_x
\]

where, \(K_n\) is the adjacency matrix of the complete graph with \(n\) vertices and \(\sigma_x\) is the Pauli matrix. Then, the Krylov bases are given by

\[
|\phi_0\rangle = |1\rangle,
|\phi_1\rangle = \frac{1}{\sqrt{n-1}}(|n+1| + |n+2| + \cdots + |2n-1|),
|\phi_2\rangle = \frac{1}{\sqrt{n-1}}(|2| + |3| + \cdots + |n|),
|\phi_3\rangle = |2n\rangle.
\]

In the above bases, the adjacency matrix is represented as

\[
A = \begin{pmatrix}
0 & \sqrt{n-1} & 0 & 0 \\
\sqrt{n-1} & 0 & n-2 & 0 \\
0 & n-2 & 0 & \sqrt{n-1} \\
0 & 0 & \sqrt{n-1} & 0
\end{pmatrix}.
\]

Again, by using (2.13) and (3.23) one can easily calculate the roots \(x_i\) and the quantities \(A\) and \(B\) as follows:

\[
x_0 = -(n-1), \quad x_1 = -1, \quad x_2 = 1, \quad x_3 = (n-1),
A \cong \frac{n-2}{2n}, \quad B \cong \frac{(n-1)^2}{n^2}.
\]
Now, by using (3.25), (3.26) and (3.27), one can obtain
\[
\gamma_{\text{crit.}} \approx \frac{s}{1 - s} \sqrt{\frac{n - 1}{n^2}},
\]
\[
g_{\text{min}}(s) \approx s(1 + 2 \sqrt{\frac{(n - 2)(n - 1)^2}{n^2}}),
\]
\[
T \approx \frac{1}{\epsilon \left(1 + 2 \sqrt{\frac{(n - 2)(n - 1)^2}{n^2}}\right)^2} \approx \frac{1}{\epsilon n}.
\]

5 Conclusion

Based on the local adiabatic evolution of the Hamiltonian and some techniques such as Krylov subspace projection methods, Lanczos iteration algorithm and spectral distribution methods, a new procedure for investigating quantum search in the state space of a graph was introduced, where an approximate analytical formula for calculating the corresponding minimum energy gap and the total search time was given.

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