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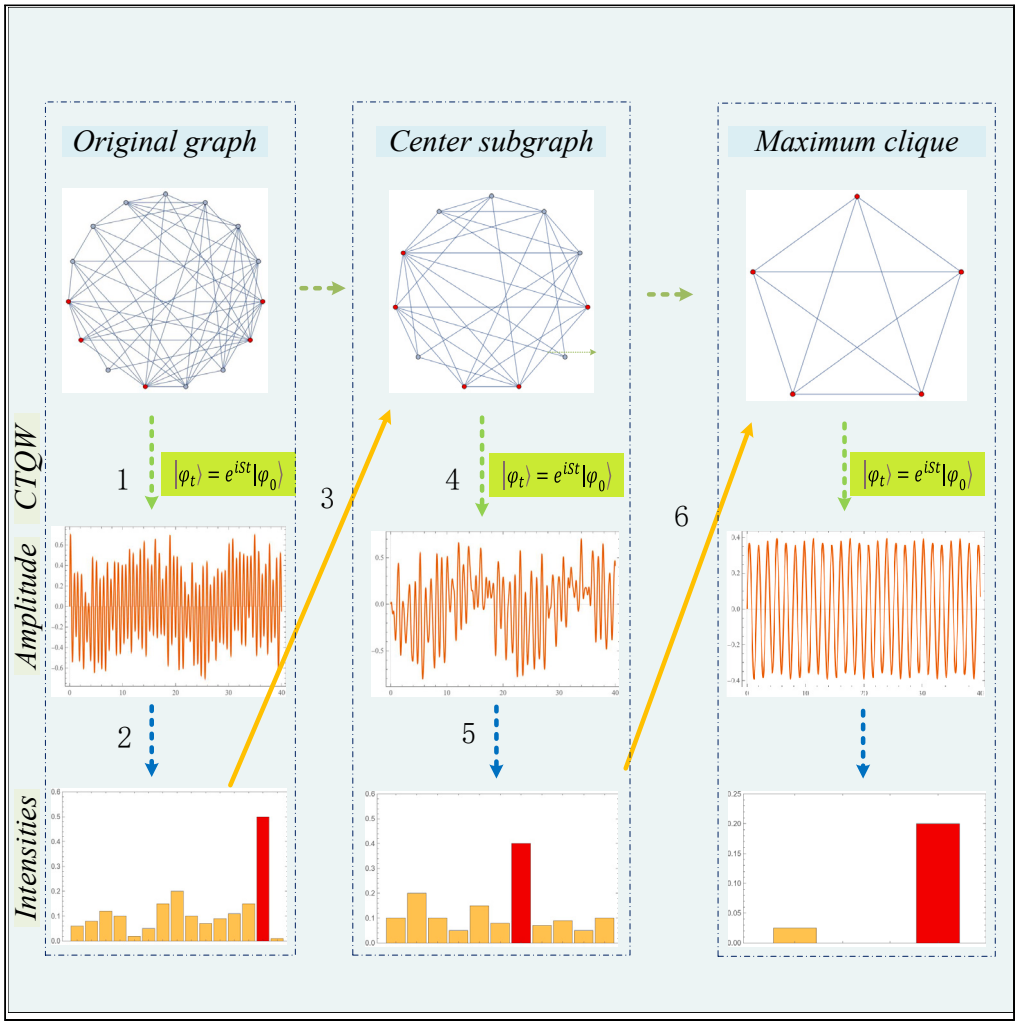

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Highlights

Present a parameter-independent quantum-based algorithm for finding maximum clique

Demonstrated the correlation of clique structure and Seidel quantum walk

Give several inequalities for four type of graph on amplitudes of CTQW

Compared the algorithm with CTQW to the simulated quantum evolution algorithm

Li et al., iScience 27, 108953
February 16, 2024
https://doi.org/10.1016/j.isci.2024.108953

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A parameter-independent algorithm of finding maximum clique with Seidel continuous-time quantum walks

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SUMMARY

The maximum clique (MC) problem holds significance in network analysis. Quantum-based algorithms have recently emerged as promising approaches for this problem. However, these algorithms heavily depend on parameters of quantum system and vary significantly for different graphs. In order to tackle this issue, we initially demonstrate that continuous-time quantum walks (CTQW) driven by the Seidel matrix offer valuable insights into the clique structure of graphs, outperforming the CTQW driven by adjacency matrix. Specifically, we conduct an in-depth analysis for CTQW of 4 types of graphs, meticulously calculating the amplitudes associated with different vertices. Our findings consistently reveal that vertices belonging to MC exhibit the highest intensity at the largest frequency component of the probability amplitude for these types of graphs. Considering the varying intensities, we propose a parameter-independent algorithm for determining the MC. We compare our algorithm with a typical quantum-based algorithm, the results indicate that our algorithm exhibits greater stability.

INTRODUCTION

The problem of determining the maximum clique (complete subgraph) in a given graph holds significant practical relevance in various fields. For instance, it plays a crucial role in network coding,[1] protein structure alignment,[2] and social network analysis.[3] It's worth noting that finding the maximum clique (MC) is a well-known non-deterministic polynomial complete problem (NP-complete problem).[4,5] Exact algorithms for this problem have a time complexity of $O(2^{0.249N})$[6], making them impractical for graphs with large cardinality. Consequently, heuristic algorithms, such as sequential greedy heuristics, are commonly used to approximate the solution.[7] These heuristics iteratively build a maximal clique by adding or removing vertices until a maximal clique is found. To enhance the quality of the solution provided by sequential greedy heuristics, local search heuristics explore the neighborhood of the maximal clique. The k-interchange heuristics, based on the k-neighbor of a feasible solution, are a well-known example.[8] However, traditional local search heuristics often find only locally optimal solutions. To mitigate this issue, advanced search heuristics like tabu search,[9] simulated annealing,[10] and neural network-based algorithms[11] have been proposed to reduce the risk of falling into local optimality. Some strategies may help improve the heuristics,[12,13] in which the auxiliary parameters or functions are still necessary. Classical heuristic algorithms struggle with large graphs, facing challenges like exponential search space growth, local optima traps, and high resource demands. These limitations motivate the exploration of quantum-inspired heuristics for more effective solutions in handling complexities of large-scale graph problems.

Quantum algorithms have demonstrated their superiority over classical algorithms in various applications.[14–17] This has prompted scientists to explore their potential for solving NP-complete problems.[18–21] The quantum adiabatic algorithm (QAA) is a universal quantum algorithm frequently used for combinatorial optimization problems.[22] In QAA, quantum systems evolve adiabatically from an initial state to a final state encoded as the solution of the problem, driven by a time-dependent Hamiltonian. QAA-based algorithms have shown promise for finding k cliques in graphs[23] and outperforming simulated annealing for larger random graphs.[24] Additionally, the quantum approximate optimization algorithm (QAOA), an approximation of QAA, can be simulated on classical computers. However, both QAA and QAOA face limitations when dealing with large-sized graphs due to constraints on qubit numbers or the computational challenges of exponential matrices. Numerically simulating adiabatic evolutions (SAE) of classical nonlinear systems exhibiting bifurcation phenomena can handle this problem, so it can be used to combinatorial optimization problems[25,26] with larger scale. But the results of SAE still depend on the density of edges, and multiple system parameters which are not easy to select.

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https://doi.org/10.1016/j.isci.2024.108953

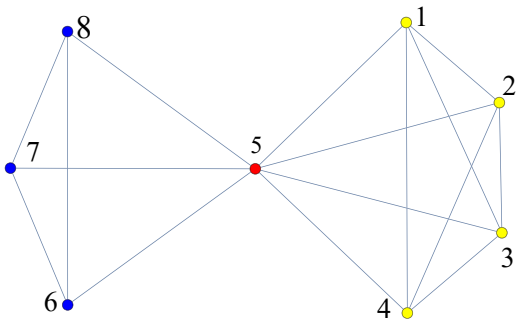

Figure 1. An instance of the first kind of ideal center graph

Vertex 5 is the center vertex. Within the graph, two distinct cliques are present. The first clique is the subgraph with the vertex set of {1,2,3,4,5}, while the second clique forms a subgraph with the vertex set of {5,6,7,8}. Aside from the center vertex 5, there are no edges connecting the two cliques.

Unlike other quantum algorithms, quantum walks aim to solve problems by obtaining a desirable probability distribution[27–33] or comparing the probability amplitudes of two walking systems.[34,35] In this study, we investigate the probability amplitudes of continuous-time quantum walks (CTQW) on several special graphs and use these amplitudes to deduce a clique within the given graph. In the initial version of CTQW, the adjacency matrix, or Laplacian matrix of the graph is commonly used as the driving Hamiltonian. Consequently, probability amplitudes naturally imply the position of the clique in some special graphs. However, we will demonstrate that the Seidel matrix serves as a more effective driving Hamiltonian for obtaining information about the MC. Therefore, the CTQW is defined as $|\varphi(t)\rangle = e^{iHt}|\varphi(0)\rangle$ in this work, where H is taken to be the Seidel matrix or adjacency matrix of the given graph G. Furthermore, we will illustrate how CTQW reflects the clique structures of several types of graphs, specifically how the probability amplitude of a vertex in the graph indicates its membership in the MC. And then put forward an algorithm based on CTQW to find the MC. Finally, we will compare our algorithm with the SAE algorithm, and the results show that our algorithm is more stable.

RESULTS

Inequalities for four types of ideal center graphs

The first kind of ideal center graph

A graph G_j is characterized as the first kind of ideal center graph if it contains two cliques and no edges exist between any pair of vertices v_k, v_l, where v_k and v_l are members of distinct cliques. An example of the first kind of ideal center graph is shown in Figure 1.

When considering the Seidel matrix as a directed adjacency matrix, the walks within the corresponding directed graph become directed walks. These counts of weighted walks can be determined by utilizing recursion equations. To provide a more detailed explanation, let W_ζ represent the number of closed walks of length ζ originating from the center vertex. Similarly, F_ζ denotes the number of walks of length ζ starting at the center vertex j and terminating at one of the vertices within the MC, while H_ζ signifies the number of walks of length ζ starting from the center vertex j and concluding at one of the vertices outside the MC. Consequently, these quantities can be expressed as follows:

$$\begin{cases} W_{\zeta+1} = (m_1 - 1)F_\zeta + (m_2 - 1)H_\zeta, \\ F_{\zeta+1} = W_\zeta + (m_1 - 2)F_\zeta - (m_2 - 1)H_\zeta, \\ H_{\zeta+1} = W_\zeta + (m_2 - 2)H_\zeta - (m_1 - 1)F_\zeta. \end{cases} \quad \text{(Equation 1)}$$

Where m_1 is the size of the MC and m_2 is the size of the remaining clique. The exact solutions are complex and do not help to infer whether a vertex belongs to the MC or not. Moreover, the relationships between the probability amplitudes of different vertices are only needed. Thus, referring to the literature results,[36,37] we have

$$W_\zeta = \sum_{n=1}^{N} a_n \lambda_n^\zeta, \quad \text{(Equation 2)}$$

where $\sum_{n=1}^{N} a_n = 1$. Combining Equation 2 and Equation 1, we have

$$F_\zeta = \sum_{j=1}^{N} \frac{\alpha_j(\lambda_j - 1)\lambda_j^\zeta}{2m_1 - 3 - \lambda_j}, \quad \text{(Equation 3)}$$

and

$$H_\zeta = \sum_{j=1}^{N} \frac{\alpha_j(\lambda_j - 1)\lambda_j^\zeta}{2m_2 - 3 - \lambda_j}. \quad \text{(Equation 4)}$$

From the perspective of exponential function, the amplitude of CTQW can be expressed in a summation form,

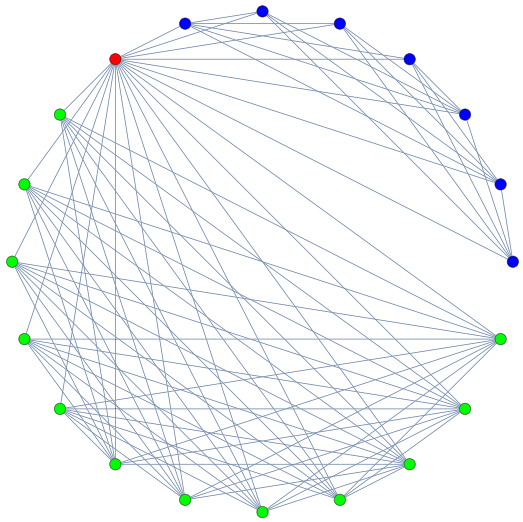

Figure 2. An example of second kind of ideal center graph
The red vertex is the center vertex, the blue vertices and the green vertices consist of two complete multipartite graph ($K_{2,3,2}$ and $K_{3,4,5}$), respectively.

$$\alpha_{l,j}(t) = \sum_{\zeta=0}^{\infty} \frac{(it)^{\zeta}(S^{\zeta})_{l,j}}{\zeta!}. \quad \text{(Equation 5)}$$

Where $(S^{\zeta})_{l,j}$ is the number of directed walks from vertex v_l to v_j. Hence, the probability amplitude of v_l, which is a vertex of MC, is represented as follows:

$$\alpha_{l,k}(t) = \sum_{j=1}^{N} \frac{\alpha_j(\lambda_j - 1)e^{i\lambda_j t}}{2m_1 - 3 - \lambda_j}, \quad \text{(Equation 6)}$$

and, when v_k is not a member of the MC, the probability amplitude can be expressed as follows:

$$\alpha_{l,k}(t) = \sum_{j=1}^{N} \frac{\alpha_j(\lambda_j - 1)e^{i\lambda_j t}}{2m_2 - 3 - \lambda_j}. \quad \text{(Equation 7)}$$

Let $p_{l,n} = \left|\frac{1}{2m_1 - 3 - \lambda_n}\right|$ be the intensity of the amplitude at the λ_1 frequency component, namely it denotes the coefficient of $\alpha_{l,j}$ at eigenvalue λ_n, then the following inequality is satisfied, it can be seen in the SUPPLEMENTAL INFORMATION,

$$\left|p_{l,1}\right| > \left|p_{k,1}\right|, \quad \text{(Equation 8)}$$

i.e.,

$$\left|\frac{1}{2m_1 - 3 - \lambda_1}\right| > \left|\frac{1}{2m_2 - 3 - \lambda_1}\right|. \quad \text{(Equation 9)}$$

The second kind of ideal center graph

A center graph G_j is classified as the second kind of ideal center graph, if G_j contains multiple complete multipartite subgraphs, and there are no edges connecting vertices between these subgraphs. An illustrative example of a graph falling into this category is depicted in Figure 2.

Let $m_1 - 1$ and $m_2 - 1$. is the number of independent sets of the two complete multipartite subgraphs, with $m_2 < m_1$. With this configuration, the size of the MC is m_1. Then the probability amplitude of v_k, which is a vertex of MC, is denoted as follows

$$\alpha_{l,k}(t) = \sum_{j=1}^{N} \frac{\alpha_j(\lambda_j - 1)e^{i\lambda_j t}}{(2m_1 - 4)\,z{+}1 - \lambda_j}, \quad \text{(Equation 10)}$$

when v_k is not a member of the MC, the probability amplitude is equal to

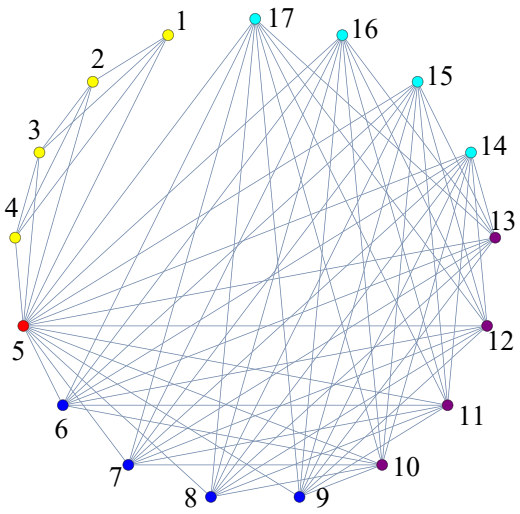

Figure 3. An instance of the third kind of ideal center graph

The subgraph induced by $\{1, 2, 3, 4, 5\}$ is the maximum clique with size 5. The subgraph induced by vertices $\{6, 7, \ldots, 17\}$ is a complete 3-partite graph, where vertices in the same independent set share the same color. There are no edges connecting the vertices in the MC and those not in the MC.

$$\alpha_{l,k}(t) = \sum_{j=1}^{N} \frac{\alpha_j(\lambda_j - 1)e^{i\lambda_j t}}{(2m_2 - 4)\,z+1 - \lambda_j}. \quad \text{(Equation 11)}$$

Referring to the SUPPLEMENTAL INFORMATION, we have:

$$\left|p_{l,1}\right| > \left|p_{k,1}\right|, \quad \text{(Equation 12)}$$

i.e.,

$$\left|\frac{1}{(2m_1 - 4)\,z+1 - \lambda_1}\right| > \left|\frac{1}{(2m_2 - 4)\,z+1 - \lambda_1}\right|. \quad \text{(Equation 13)}$$

where v_l is a member of the MC, and v_k is a vertex of the remaining clique.

The third kind of ideal center graph

A center graph G_j is categorized as the third kind of ideal center graph when it contains an MC denoted as Γ and a complete multipartite subgraph designated as H, with no edges connecting these two subgraphs. As an example, Figure 3 shows a graph of this type.

Consider the case where there are $m_2 - 1$ independent set in the complete multipartite subgraph, and $(m_2 - 2)z > m_1$. Then the probability amplitude of a member of MC is determined as follows:

$$\alpha_{l,k}(t) = \sum_{j=1}^{N} \frac{\alpha_j(\lambda_j - 1)e^{i\lambda_j t}}{2m_1 - 3 - \lambda_j}, \quad \text{(Equation 14)}$$

and for a vertex that does not belong to the MC, it is defined as follows:

$$\alpha_{l,k}(t) = \sum_{j=1}^{N} \frac{\alpha_j(\lambda_j - 1)e^{i\lambda_j t}}{2m_2 z - 4z+1 - \lambda_j}. \quad \text{(Equation 15)}$$

With similar definition of $p_{l,n}$, the following inequality is approximately satisfied, it can be seen in the SUPPLEMENTAL INFORMATION,

$$\left|p_{l,1}\right| > \left|p_{k,1}\right|, \quad \text{(Equation 16)}$$

namely:

$$\left|\frac{1}{2m_1 - 3 - \lambda_1}\right| > \left|\frac{1}{2m_2 z - 4z+1 - \lambda_j}\right|. \quad \text{(Equation 17)}$$

It is worth mentioning that if the adjacency matrix A is the Hamiltonian, then the we have contrary conclusion referring to Equation 17 if z is big enough, i.e.,

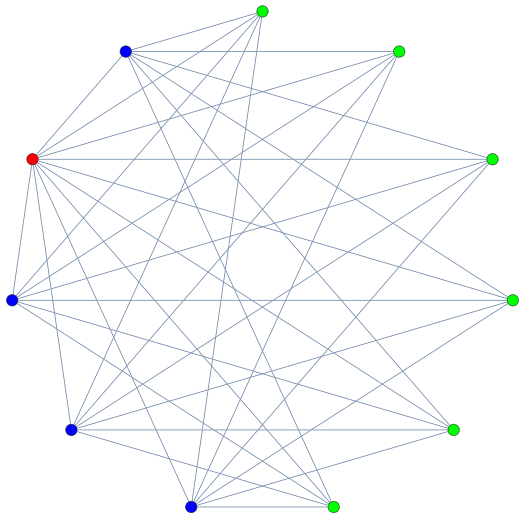

Figure 4. An instance of the fourth kind of ideal center graph

The red vertex is the center vertex, and subgraph induced by all other vertices is a complete 2-partite graph in which there are 4 and 6 vertices in each independent set.

$$\left| p_{l,1} \right| < \left| p_{k,1} \right|. \quad \text{(Equation 18)}$$

The fourth kind of ideal center graph

A center graph G_j is called the fourth kind of ideal center graph if it only contains a center vertex and a complete multi-partite subgraph H. Generally, the number of vertices in each independent sets of H is not equal. And a center vertex is connecting to all vertices of H. For the instance showed in Figure 4, H is a complete 2-partite subgraph and there are 4 and 6 vertices in these two independent sets, respectively.

For the instance where H is a complete 2-partite subgraph and there are r_1 and $r_2 (r_2 > r_1)$. vertices in these two independent sets. For a vertex that does not belong to the largest independent set, the amplitude is:

$$\alpha_{l,k}(t) = \sum_{j=1}^{N} \frac{\alpha_j (\lambda_j + 1) e^{i\lambda_j t}}{2r_1 + \lambda_n - 1}, \quad \text{(Equation 19)}$$

d the probability amplitude of a vertex in the largest independent sets:

$$\alpha_{l,k}(t) = \sum_{j=1}^{N} \frac{\alpha_j (\lambda_j + 1) e^{i\lambda_j t}}{2r_2 + \lambda_n - 1}. \quad \text{(Equation 20)}$$

For $0 < r_1 < r_2$, it is clear that $0 < 2r_1 + \lambda_1 - 1 < 2r_2 + \lambda_1 - 1.$, therefore, we have

$$\left| \frac{1}{2r_1 + \lambda_1 - 1} \right| > \left| \frac{1}{2r_2 + \lambda_1 - 1} \right|. \quad \text{(Equation 21)}$$

Results of algorithm with CTQW on random graphs

Based on the four inequalities in the previous subsection, we have designed Algorithm 1 (see the supplemental information) for finding the MC with CTQW. And then we tested our algorithm on random graphs, and the results are shown in Figure 5. The sizes of graphs ranging from order 20 to 100 are provided, with 10,000 random graphs sampled for each order, and the corresponding average clique sizes are plotted on the horizontal axis. In the numerical experiments, we also verified the clique numbers of every graph using the classical exact algorithm, branch-and-bound method. The curves in Figure 5 demonstrate a trend converging to $\log(N)$, which aligns with random graph theory.[38] This observation illustrates the high accuracy of our algorithm.

Simulating adiabatic bifurcations (SAB) in nonlinear Hamiltonian systems is a typical quantum-based algorithm for combinatorial optimization.[26] We have compared its performance with our algorithm by applying them to the same set of graphs. The results are presented in Table 1, where $G(N,p), p < 1$, represents random graphs with N vertices and an edge existence probability of p. The numbers in the table represent the mean values of clique sizes.

Both of these algorithms were employed to find the MC in random graphs with varying values of p. The results indicate that both algorithms perform well for $G(50, 0.3)$ and $G(100, 0.3)$. However, the algorithm utilizing CTQW consistently identifies larger cliques than the

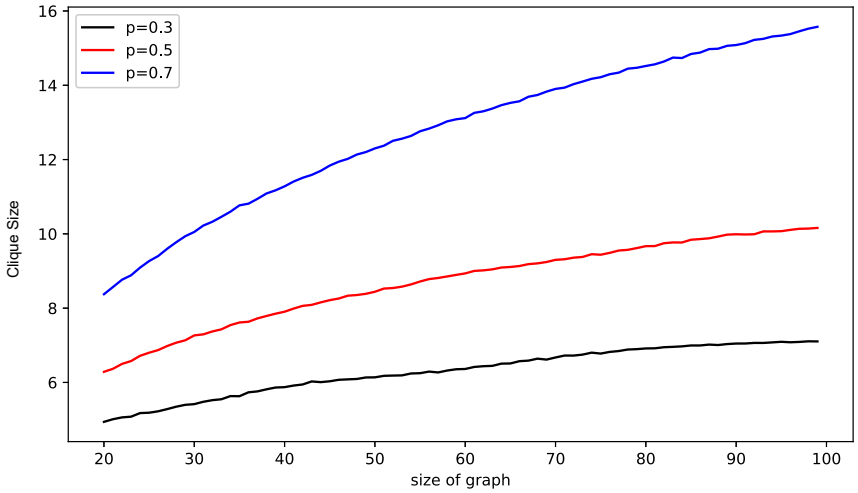

Figure 5. Experimental results of the algorithm on random graphs

The horizontal axis refers to the size of the graph, and the vertical axis corresponds the expected size of clique number.

SAB-based algorithm as the edge existence probability changes. It's worth noting that the SAB-based algorithm may require multiple executions to determine the MC, and the parameter should be adjusted for each time, since it depends on several parameters and the initial state of the quantum system. As a result, the algorithm with CTQW is parameter-independent and more stable for varying p.

DISCUSSION

In this paper, we demonstrate a profound relationship between the clique structure of a graph and CTQW driven by the Seidel matrix. We provide a detailed analysis of the intensity relations observed in CTQW on four distinct types of center graphs. Specifically, we find that clique vertices exhibit a higher intensity in CTQW at the largest eigenvalue. Consequently, the intensity of the probability amplitude in CTQW serves as a valuable feature for directly determining whether a vertex belongs to the MC in these four graph types.

Given that the eigenvalues of the Seidel matrix correspond to the frequencies of CTQW, we establish a connection between the clique structure and these eigenvalues and their corresponding eigenvectors. However, for general graphs, this feature is not readily apparent, and identifying the MC directly becomes a challenging task. To unveil the concealed MC in such graphs, we propose an innovative CTQW-based algorithm, denoted as Algorithm 1, which exhibits a time complexity of less than $O(N^4 \log(N))$. Our algorithm has been rigorously tested through numerical experiments on random graphs, demonstrating its efficacy.

Furthermore, we assess its performance by comparing it with another quantum-based algorithm, the SAB-based algorithm, across random graphs with varying edge existence probabilities. The findings indicate that our algorithm demonstrates enhanced stability and parameter-independence, consistently identifying larger cliques. The SAB-based algorithm directly employs quantum evolution, resembling the characteristics of quantum annealing, where the occurrence of getting stuck in a local optimal solution is a common phenomenon. We believe this is because the algorithm only relies on local information to search for maximal cliques. Actually, similar with the SAB-based algorithms, the algorithms that only rely on partial information may exhibit varying performance across different graphs. For instance, the degree sequence is frequently employed as a heuristic, either directly or indirectly. Degrees can be viewed as the count of closed walks of length 2 from the perspective of the adjacency matrix, and this information can be derived from the square of the adjacency matrix. In contrast, our algorithm utilizes the amplitude in CTQW. Considering the counts of walks of all lengths increases the likelihood of identifying specific vertices. The n-th power of the adjacency matrix and Seidel matrix provides counts of walks and directed walks of length n. These two types of CTQW complement each other, allowing one to handle challenging instances where the other may struggle.

Limitations of the study

There are some limitations in our study. These limitations of improvement encompass three key aspects. Firstly, new methods for mitigating the time costs associated with our methodology needs to be studied in future. The main work is to explore strategies that reduce or circumvent the need for numerical estimation of the largest eigenvector, a process that currently incurs a significant time complexity of N^2. Secondly, more endeavors for delving deeper into the relationships between CTQW and the clique structures of graphs is needed, since the types of graphs grow rapidly as the problem size increases. In pursuit of this objective, we intend to investigate the probability amplitude characteristics of CTQW across a broader range of graph types. This expanded analysis aims to unearth valuable insights that can facilitate the deduction of MCs. Furthermore, the exploring on the connections between the probabilities generated by CTQW and the underlying clique structures is needed. Given that quantum system probabilities can be ascertained through measurements, this approach holds promise for further elucidating the relations between quantum dynamics and clique identification.

Table 1. Our algorithm Vs. SAB-based algorithm

Random graphs	$G(50,0.3)$	$G(50,0.5)$	$G(50,0.7)$
SAB-based algorithm	5.11	7.5	11
Ours	5.11	7.513	11.3125
Random graphs	$G(100,0.3)$	$G(100,0.5)$	$G(100,0.7)$
SAB-based algorithm	6.1875	8.8125	13.75
Ours	6.1875	9.19	14.5

STAR★METHODS

Detailed methods are provided in the online version of this paper and include the following:

- KEY RESOURCES TABLE
- RESOURCE AVAILABILITY
  - Lead contact
  - Materials availability
  - Data and code availability
- EXPERIMENTAL MODEL AND SUBJECT DETAILS
- METHOD DETAILS
- QUANTIFICATION AND STATISTICAL ANALYSIS

SUPPLEMENTAL INFORMATION

Supplemental information can be found online at https://doi.org/10.1016/j.isci.2024.108953.

ACKNOWLEDGMENTS

This work is supported by the National Natural Science Foundation of China (grant nos. 61871120 and 62071240), Natural Science Foundation of Jiangsu Province, China (grant nos. BK20191259 and BK20220804), Innovation Program for Quantum Science and Technology (grant no.2021ZD0302901) and the Six Talent Peaks Project of Jiangsu Province (grant no. XYDXX-003), Jiangsu Funding Program for Excellent Postdoctoral Talent.

AUTHOR CONTRIBUTIONS

X.L. and Z.L. designed the study. X. C., X.L., and S.H. conducted the analysis and drafted the manuscript. X.C. and J.X. finished the numerical experiments. X.L. and Z.L. revised the manuscript. All authors were involved in the data conception and the interpretation of the results. All authors reviewed and approved the final version of the manuscript.

DECLARATION OF INTERESTS

The authors declare no competing interests.

Received: October 20, 2023
Revised: January 2, 2024
Accepted: January 15, 2024
Published: January 18, 2024

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STAR★METHODS

KEY RESOURCES TABLE

REAGENT or RESOURCE	SOURCE	IDENTIFIER
Software and algorithms		
MATLAB	MathWorks	https://de.mathworks.com
Python	Python.org	https://docs.python.org/zh-cn/3/

RESOURCE AVAILABILITY

Lead contact

Further information and requests for resources and reagents should be directed to and will be fulfilled by the lead contact Xi Li (101300175@seu.edu.cn) and Zhihao Liu (liuzhtopic@163.com).

Materials availability

This study did not generate new materials.

Data and code availability

- All data reported in this paper will be shared by the lead contact upon request.
- This paper does not report original code.
- Any additional information required to reanalyze the data reported in this paper is available from the lead contact upon request.

EXPERIMENTAL MODEL AND SUBJECT DETAILS

Our study does not use experimental models typical in the life sciences.

METHOD DETAILS

The method details refers to the algorithm with CTQW for finding the maximum clique, it can be seen in the supplemental file named as "Method details".

QUANTIFICATION AND STATISTICAL ANALYSIS

We apply our algorithm and the SAE-based algorithm to the random graphs generated by Python. If the algorithm find a non-maximum clique, then it has smaller clique size. Therefore, our strategy of quantification and statistical analysis is to verify whether the maximum clique is found or check the average of clique size. The the average of the clique size by the algorithm by using CTQW is given in Figure 5. And Table 1 is the comparison between our algorithm and the SAE-based algorithm.