Spatial search with multiple marked vertices is optimal for almost all queries and its quantum advantage is not always guaranteed

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We contribute to fulfill the long-lasting gap in the understanding of the spatial search with multiple marked vertices. The theoretical framework is that of discrete-time quantum walks (QW), i.e. local unitary matrices that drive the evolution of a single particle on the lattice. QW based search algorithms are well understood when they have to tackle the fundamental problem of finding only one marked element in a $d$-dimensional grid and it has been proven they provide a quadratic advantage over classical searching protocols. However, once we consider to search more than one element, the behaviour of the algorithm may be affected by the spatial configuration of the marked elements, due to the quantum interference among themselves and even the quantum advantage is no longer granted. Here our main contribution is twofold: (i) we provide strong numerical evidence that spatial configurations are almost all optimal; and (ii) we analytically prove that the quantum advantage with respect to the classical counterpart is not always granted and it does depend on the proportion of searched elements over the total number of grid points $\tau$. We finally providing a clear phase diagram for the QW search advantage with respect to the classical random algorithm.

INTRODUCTION

One of the main applications of quantum computing is algorithmics. Considered to be still beyond the reach of today’s quantum computers, it has had a major impact in several fields, from cryptography [1] and quantum machine learning [2] to quantum simulation [3]. The first quantum algorithms were formulated in the early 1990s [4, 5], and since then researchers have continued to create new ones over the past 30 years [6], trying to optimise computing time and quantum resources. However, compared to the thousands of non-quantum algorithms, the number of quantum algorithms is still modest. This is essentially due to the difficulty of proving the advantage that each of them has over its classical counterpart. An example is given by one of the most studied problem in computer science: the quantum search in an unstructured set of $N$ elements. The first algorithm was introduced by L. K. Grover [7]. The basic idea was to introduce a quantum oracle, which recognizes a solution to a search problem when it sees one. The Grover algorithm could solve this problem in $O\left(\sqrt{N}\right)$ time, i.e. quadratically faster than what a classical computer needs to complete the same task, and it soon seemed to be extraordinary advantageous to speed-up many classical algorithms that use search heuristic [8–10]. In fact the Grover search algorithm can be applied to any decision problems whose solutions can be checked efficiently [11], with a clear polynomial speed-up. Such quantum advantage has been been proven for several generalizations, for instance when the target elements are multiple [12]. However, the situation is dramatically different for spatial searching, where quadratic speed-up is known to be possible only for some specific case. Spatial search may come in different forms, in continuous time and discrete time. The first example of spatial search algorithm in continuous time has been introduced by Childs and Goldstone [13] in the quantum walk framework, where the searching method involves now a Hamiltonian defined over an arbitrary graph, which has to be able to solve the searching problem. In this context, it has been proven that only for some certain graphs, such as a complete graph or the hypercube, the hitting time shows a quadratic speed-up respect to the classical counterpart. This long-standing problem has been recently addressed by Chakraborty, Novo and Roland [14], who obtained the necessary and sufficient conditions for the Childs and Goldstone algorithm to be optimal for any graph that meets certain general spectral properties. Another open problem that has remained poorly understood until now is the spatial search of multiple target items, both in continuous and discrete time. While the hitting time in the case we search only one target item is in line with the one recovered by the Grover algorithm, when the items are multiple, their spatial configuration can affect significantly the performance (aka the time complexity) of the algorithm. The intuitive reason behind it is that the marked vertices interfere among them, and the interplay between constructive and destructive interference may determine very different scenario. Such phenomenon has been remarked first by Aaronson and Ambainis [15] and recently observed by Bezerra et al [16], but never been studied and fully understood. Here we address this problem in the specific case of a discrete time quantum walk over a 2-dimensional grid and in this framework, we provide, for the first time, numerical evidence that almost all spatial configurations lead to an optimal success probability. Moreover, we analytically prove that the quantum advantage respect to the classical counterpart.

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depends on the proportion of searched elements over the total number of grid points \( \tau \). We provide a clear phase diagram and proving that the classical random algorithm may overtake that QW search in some specific cases.

The manuscript is organised as follows: In section I we introduce the quantum walk-based protocol in discrete time on a two dimensional square grid and the searching algorithm [23] and we shortly reviewed the analytical techniques to calculate the success probability. Then in Sec. II we carefully discuss the limits of the analytical methods in the multiple searched items framework; finally we provide numerical simulations to show how the success probability may depend on the many possible spatial configurations and we estimate a lower bound for the time complexity of the algorithm. Sec. III is devoted to investigate the quantum advantage of the QW search with multiple searched items with respect to a randomised classical algorithm. In section IV we provide a summary and some perspectives.

I. SPATIAL SEARCH ON A GRID WITH A
DISCRETE TIME QUANTUM WALK

Quantum walk can be considered the quantum counterpart of the classical Markov chain and are essentially local unitary gates that drive the evolution of a particle on a graph. However, due to quantum superposition, they are known to explore graphs faster than classical ones and in fact they have, with their beginnings in digital applications [24, 25]. Here we consider a coined QW in discrete time, defined on a square grid of size \( \sqrt{N} \times \sqrt{N} \). The walker is a complex vector \( | \psi \rangle \) living on the vertices of the grid and belonging to the composite Hilbert space \( \mathcal{H} = \mathbb{C}^2 \otimes \mathbb{Z}^2 \), where the first Hilbert space is the coin state space, spanned by the canonical basis \( \{ |0\rangle, |1\rangle \} \) and the second Hilbert space coincides with the position space spanned by \( |x, y\rangle \), with \( 0 \leq x, y \leq \sqrt{N} - 1 \). The dynamics of the walker is driven by the sequential application of a rotation in the coin state space and a shift operator, applied first along the \( x \) axis and then along the \( y \) axis as follows:

\[
U = \Sigma_y(C_y \otimes 1_N)\Sigma_x(C_x \otimes 1_N).
\]

We use two coin operators, as in [23], one for each spatial direction, whose matrix representations in the canonical basis reads:

\[
C_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \quad C_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}.
\]

The shift operator is conditioned by the coin state:

\[
\Sigma_x |\alpha\rangle |x, y\rangle = |\alpha\rangle |x - (-1)^y, y\rangle,
\]

\[
\Sigma_y |\alpha\rangle |x, y\rangle = |\alpha\rangle |x, y - (-1)^x\rangle.
\]

where \( \alpha = \{0, 1\} \). An important feature of the aforementioned QW, that has significance for its use in development of quantum algorithms, is that it is known to be efficiently implementable on a quantum computer by a circuit with a polynomial number of gates in the number of qubits. A recent example has been provided by Asif Shakeel in [26] where the circuit has linear depth and based on Quantum Fourier Transforms (QFT).

We can now solve the spatial search problem using the QW to find the marked elements \( u \in \mathcal{M} \), with \( M = |\mathcal{M}| \) the size of the marked vertices set. We recall here the idea of the algorithm as first introduced by Shenvi, Kempe and Whaley [27]: First we prepare the initial state \( |\psi(0)\rangle \) as the wave function uniformly superposed over every vertices of the grid; then we let the walker evolve with time with the quantum search operator \( U' = UR \), where \( R \) plays the role of the quantum oracle:

\[
R = 1 - 2 \sum_{u \in \mathcal{M}} |u\rangle \langle u|.
\]

Notice that, similarly to the standard oracle in the Grover algorithm, the combined action of standard quantum evolution operator \( U \) and the quantum oracle \( R \) acts by flipping the phase of the marked state. In order to find the marked state with arbitrarily small degree of error, we have to know the optimal time \( t_{\text{opt}} \) which maximise the probability to find the marked elements \( p(t) = \sum_{u \in \mathcal{M}} |\langle u|U'(t)|\psi(0)\rangle|^2 \), to measure in the computational basis and to repeat the algorithm a constant number of time. Although an exact analytical computation of the success probability for an arbitrary spatial configuration is prohibitive, Bezerra, Lugão and Portugal [16] have recently proposed an efficient method, where few assumptions are made. In short, we have to consider the subspace spanned by the eigenvectors of \( U' \), \( |\lambda\rangle \) and \( |\lambda'\rangle \), associated with the closest eigenvalues of \( U' \) to 1 and calculate the success probability as:

\[
p(t) \approx \sum_{u \in \mathcal{M}} \left| \langle u|\lambda\rangle \langle \lambda | \psi(0)\rangle e^{i\lambda t} \right|^2 + \left| \langle u|\lambda'\rangle \langle \lambda' | \psi(0)\rangle e^{i\lambda' t} + \epsilon_u \right|^2.
\]

Then, we assume the following hypothesis:

1. \( \epsilon_u \) is negligible.
2. \( \lambda = -\lambda' \).
3. \( \langle m|\lambda'\rangle \langle \lambda' | \psi(0)\rangle = -\langle m|\lambda\rangle \langle \lambda | \psi(0)\rangle \) and after simplifications the success probability \( p(t) \) reduces to:

\[
p(t) \approx 4 \sum_{u \in \mathcal{M}} |\langle m|\lambda\rangle \langle \lambda | \psi(0)\rangle|^2 \sin^2(\lambda t + c), \tag{1}
\]

where \( c \) is a constant. We refer to the above procedure as the BLP-method. Notice that the above hypothesis are fully verified if we consider only one searched element.
Then, the hitting time of this algorithm is thus
\[ p(t) = \frac{1}{4 \times 0.32 \ln(N)} \sin^2(\lambda t + c), \]
and a straightforward calculation for \( M = 1 \) leads to a
success probability:
\[ p(t) = \frac{1}{4 \times 0.32 \ln(N)} \sin^2(\lambda t + c), \]
where
\[ \lambda = \frac{2}{\sqrt{0.32N \ln(N)}} \]
and
\[ c = -2\sqrt{0.32 \ln(N)} \frac{1}{N}. \]
Then, the hitting time of this algorithm is thus
\[ t_{opt} = \frac{\pi}{4} 0.32 \sqrt{N \ln(N)} + 0.32 \ln(N). \]
Moreover, making use of quantum amplitude amplification [28], one just needs \( O(\log N) \) repetitions of the algorithm in order to make the probability an \( O(1) \), yielding an overall complexity of \( O(\sqrt{N \ln(N)})^{1/2} \). We have provided a detailed proof of the above calculations in the appendix A.

II. SEARCHING MULTIPLE MARKED VERTICES

However, whenever we consider \( M \neq 1 \), the BLP hypothesis do not hold for any cases. Bezerra, Lugão and Portugal already pointed it out but they did not precise how many spatial configurations are concerned for a given number of marked elements. How does this failure affect the spatial search? How far does the spatial search hold a quantum advantage with respect to the classical counterpart? Our numerical simulations shown in Fig. 2 strongly suggest that, although the BLP-method is not in general longer predictive, almost all of the displayed spatial configurations are still well fitted by the function \( p_{fit}(t) = A \sin^2(\lambda t + c) \). In order to be convinced of that, let us consider the simplest but not trivial case where the searching problem is solved for only two searched items, as shown in Table I. Notice that the relative position of the searched elements affects the probability distribution of the walker, that deviates from the predicted success probability according to the BLP-method (the orange curve). This may suggest a prominent role of quantum interference and its interplay with the quantum amplification on the searched elements. Indeed, the predicted frequency \( \lambda \) is no longer sufficient to foresee the behaviour of the walker and in general does not coincide with the observed frequency \( \tilde{\lambda} \). Quite interestingly, the values of \( \lambda \) in Table I are related to the first two closest eigenvalues of \( U' \) to 1, \( e^{i\lambda_1} \) and \( e^{i\lambda_2} \) and their conjugates, where \( \lambda_2 \geq \lambda_1 > 0 \). In particular, we observed that the discrepancy between the predicted \( \lambda \) and the observed \( \tilde{\lambda} \) only depends on the coefficient \( \langle u|\lambda_k \rangle \langle \lambda_k | \psi(0) \rangle \), with \( k = \{1, 2\} \). For the first configuration displayed in Fig. 2a, both eigenvalues coincide, i.e. \( \lambda_2 = \lambda_1 \), and \( \langle u|\lambda_k \rangle \langle \lambda_k | \psi(0) \rangle = (\langle u | -\lambda_k \rangle \langle -\lambda_k | \psi(0) \rangle) \). So the actual oscillation frequency is given by \( \lambda = \lambda_1 \). In this case, the BLP hypothesis hold. In Fig. 2b, the eigenvalues again coincide, \( \lambda_2 = \lambda_1 \). But the coefficients \( \langle u|\lambda_k \rangle \langle \lambda_k | \psi(0) \rangle \) and \( \langle u | -\lambda_k \rangle \langle -\lambda_k | \psi(0) \rangle \) are different, leading to two frequencies \( \{\lambda_1, \lambda_1/2\} \). The probability distribution of the QW is periodic according to \( \lambda = \lambda_1/2 \). But now the success probability displays two close peaks with frequency \( \lambda_1 \). In Fig. 2c, the observed frequency is \( (\lambda_1 + \lambda_2)/2 \), which is surprisingly almost identical to the frequency observed with a single searched element. Finally, Fig. 2d displays an intermediate case between Fig. 2c and Fig 2b, where the frequency \( \tilde{\lambda} = (\lambda_1 + \lambda_2)/2 \) and again the success probability displays two close peaks appearing at frequency \( (\lambda_1 + \lambda_2)/4 \).

The numerical data we provided suggest that the interference plays a major role to determine the success probability of the search and that an analytical calculation of the exact frequency \( \lambda \) has to take in consideration more than the first closest eigenvalue \( \lambda_1 \). However, without a general method to compute the success probability for an arbitrary number of marked elements, we do not know how many of those spatial configurations lead to an optimal search. Some of them might affect negatively the success probability, some other can even amplifies it like in Fig. 2a. Still we can count them by numerical means. We will proceed as follows: at fixed \( M \) and grid size we generate numerically 1000 spatial configurations and we count among them, the optimal ones. Here we call optimal a configuration of marked elements that leads to a success probability bounded by the bottom by
\[ p(t_{opt}) = \frac{1}{4 \times 0.32 \ln(N)} \sin^2(\lambda t + c), \]
the optimal success probability for one marked item. Then we characterise the proportion of the optimal configurations in function of \( M \).

As it is shown in Fig. 3 this proportion changes according to the number of marked elements but it is never lower than 1/2, thus the lower bound for the optimal
TABLE I: Different spatial configurations of two marked elements. The parameter $\tilde{\lambda}$ is the fitting parameter for the success probability $p_{\text{fit}}(t) = A \sin^2(\tilde{\lambda}t + c)$ showed in Fig. 2.

FIG. 2: The probability of success $p(t)$ after $t$ steps for a few configurations of two marked elements. The details of the configurations are listed in table I.

FIG. 3: Proportion of winning configurations depending of the number of marked elements $M$.

FIG. 4: Average probability of success over the marked elements’ configurations.

success probability, for $M > 1$ reads

$$p_{\text{lower}}^{\text{lower}}(t_{\text{opt}}) \geq \frac{1}{8 \times 0.32 \ln(N)}.$$

Notice that the overall complexity of the spatial algorithm does not change with the number of marked vertices like the Grover’s algorithm does. The success probability averaged over all spatial configurations is shown in Fig. 4 and it is always larger than the one marked element case. In conclusion, notice that both the proportion of winning configurations and the average success probability increase significantly with the number of marked element. This is expected since the more marked elements means the higher success probability.

III. QUANTUM ADVANTAGE

In this last section we now aim to see how far does the spatial search still hold a quantum advantage respect to
the classical counterpart when multiple marked vertices are considered. Thus we introduce a classical randomised search algorithm and we compare the time complexities in both cases, quantum and classical. The key idea behind the classical randomized search algorithm is basically to sample one element of the grid according to an uniform distribution. The success probability is simply given by the ratio \( \tau = M/N \) while the complexity time is \( O(1) \). In order to compare both algorithms, we repeat the classical one a logarithmic number of time steps. Thus, the success probability for the amplified classical randomised search algorithm reads

\[
p_{\text{classic}} = \frac{1}{8 \times 0.32 \ln(N)}
\]

and the overall optimal time is given by

\[
T_{\text{classic}} = \frac{\ln\left(\frac{1}{8 \times 0.32 \ln(N)}\right)}{\ln(1 - \tau)}.
\]

Notice that if we increase the number of elements \( N \), keeping the same ratio \( \tau \), we end up with a classical randomized algorithm faster than the QW search. This is illustrated in Fig. 5 where we can see that, although the QW search algorithm displays a neat quantum advantage for small dataset’s sizes \( N \), the classical randomized algorithm is faster for large \( N \). Moreover, we compute the crossing point between the two curves of Fig. 5 and we determine the critical size \( N_c \) for which the classical randomized algorithm overtakes the QW search. The phase diagram in Fig. 6 shows this value in function of \( \tau \). As expected, the smaller the ratio \( \tau \), the longer the QW search holds the advantage.

IV. DISCUSSION

Quantum walk search algorithm for a two dimensional square grid is well understood when the searched item is single. However when the searched items are multiple there is not a full general method to compute the success probability. The recent BLP method holds for some specific case, in particular when the calculation of the success probability depends on the closest eigenvalue to 1 of the searching operator \( U' \). However in all other cases numerical techniques are the only possible mean. Starting from the simplest but not trivial case of two searched items, we first numerically provided evidence how their location on the grid can affect drastically the probability distribution of the walker and then we show that by relaxing the hypothesis of the BLP method, we can recover the exact success probability of such cases. To the best of our knowledge, the idea that spatial location of the searched items can affect the success probability of the search has been poorly remarked in the past and never investigated. Moreover, by means of large scale numerical simulation, we proved that most of spatial configurations of the search items, leads to an optimal success probability. Furthermore, differently from the standard Grover algorithm, the hitting time of the algorithm does not depend of the number of marked elements. We concluded our study arguing that the QW search does not always display quantum advantage with respect to the classical algorithm. In order to prove it, we introduced a randomised algorithm and computed analytically a phase diagram showing that the classical randomized algorithm overtakes the QW search algorithm for certain values of \( \tau = M/N \), the proportion of the searched elements over the size of the grid, and \( N \). Finally, the complexity of this algorithm slightly improves the quantum spatial search alternative proposed by Aaronson and Ambainis [15], where Grover’s quantum robots are introduced on the grid to

FIG. 5: Hitting time of the QW search algorithm and the classical randomized algorithm in function of the dataset’s size \( N \) where \( \tau = 0.01 \).

FIG. 6: Number of elements after which it is more advantageous to use a classical randomized algorithm over the QW search in function of the proportion of searched elements \( \tau = M/N \).
search marked elements. Indeed such an algorithm has an overall time complexity, after quantum amplification, equals to $O(\sqrt{N} \ln(N)^{5/2})$ versus $O(\sqrt{N} \ln(N)^{3/2})$, displayed by the QW search.

A more in-depth and rigorous study of how configurations affect the probability of success of the algorithm and in particular, an effective method to calculate the time complexity from an arbitrary configuration is one of the next directions of research. Furthermore, a study on how certain spatial configurations are more resilient to errors is another open question we would like to address in the future.

**Appendix A: Analytical solution for one elements**

The purpose of this section is to further detail the analytical analysis of the QW Search algorithm for one single element in a data set of $N = n^2$ elements. We assume that the marked element is 0 for the computations without loss of generality. In short we have to

1. compute the eigenvalues $e^{i \phi_k}$ of $U$ and the corresponding eigenvectors $| \psi_k \rangle$;
2. consider the $M \times M$ matrix $A_{m,m'} = \sum_k b_k^\lambda \langle m | \psi_k \rangle \langle \psi_k | m' \rangle$, where $b_k^\lambda = \sin(\lambda - \phi_k) / (1 - \cos(\lambda - \phi_k))$;
3. solve the equation $\det(A^\lambda) = 0$, to compute $\lambda$;
4. solve the equation $A^\lambda \psi = 0$ where $\psi_m = \langle m | \lambda \rangle$, to recover $\langle m | \lambda \rangle$;
5. calculate $\langle \psi_k | \lambda \rangle = (1 + i b_k^\lambda) \sum_m \langle \psi_k | m \rangle \langle m | \lambda \rangle$, which yields $\langle \psi_k | \lambda \rangle$.

### 1. Spectral analysis of $U$

In the following, the eigenvectors $\psi_{\pm, k,l}$ and corresponding eigenvalues $e^{i \phi_{\pm, k,l}}$ will be indexed by $\pm, k \in \{0, \ldots, n - 1\}, l \in \{0, \ldots, n - 1\}$. We also define $\omega = e^{2 \pi i/n}$.

The eigenvector $\psi_{\pm, k,l}$ is of the form

$$
\psi_{\pm, k,l} = |v_{\pm, k,l} \rangle \otimes \frac{1}{n} \sum_{x,y=0}^{n-1} \omega^{kx + ly} |x,y\rangle.
$$

The form of $v_{\pm, k,l}$ does not need to be explicit in the following but the eigenvalue associated to $\psi_{\pm, k,l}$ does.

Let us look at $U | \psi_{\pm, k,l} \rangle$

$$
U | \psi_{\pm, k,l} \rangle = C | v_{\pm, k,l} \rangle \otimes \frac{1}{n} \sum_{x,y=0}^{n-1} \omega^{kx + ly} |x,y\rangle,
$$

where

$$
C = \begin{pmatrix}
\omega^l \cos \left(\frac{2\pi k}{n}\right) & \omega^l \sin \left(\frac{2\pi k}{n}\right) \\
\omega^{-l} \sin \left(\frac{2\pi k}{n}\right) & \omega^{-l} \cos \left(\frac{2\pi k}{n}\right)
\end{pmatrix}.
$$

The eigenvalues are $e^{i \phi_{\pm, k,l}}$ where

$$
\phi_{\pm, k,l} = \pm \arccos \left(\frac{\cos \left(\frac{2\pi k}{n}\right) \cos \left(\frac{2\pi l}{n}\right)}{\sin \left(\frac{2\pi}{n}\right)}\right).
$$

### 2. Estimation of $\lambda$ and the coefficients

Now we try to estimate the eigenvalue $e^{i \lambda}$ with $\lambda > 0$ as close as possible to 0. We define

$$
\lambda^\lambda = \sum_{\pm, k,l} b_{\pm, k,l}^\lambda,
$$

where

$$
b_{\pm, k,l}^\lambda = \frac{\sin(\lambda - \phi_{\pm, k,l})}{1 - \cos(\lambda - \phi_{\pm, k,l})}.
$$

We want to solve $\lambda^\lambda = 0$ which will yield the value of $\lambda$. First, we note that

$$
b_{\pm, k,l}^\lambda = \begin{cases}
\frac{2}{\lambda} & \text{if } \phi_{\pm, k,l} = 0 \\
\frac{1}{\cos(\phi_{+ k,l}) - 1} & \text{otherwise}
\end{cases},
$$

where

$$
a_{k,l} = \frac{1}{\cos(\phi_{+ k,l}) - 1}.
$$

We can thus cut $\lambda^\lambda$ into three sums.

$$
\lambda^\lambda = \frac{1}{\lambda} A + B - \lambda C,
$$

where

$$
A = \sum_{\pm, k,l, \phi_{\pm, k,l} = 0} 1,
$$

and

$$
B = \sum_{\pm, k,l, \phi_{\pm, k,l} \neq 0} a_{k,l} \sin(\phi_{\pm, k,l}),
$$

and

$$
C = \sum_{\pm, k,l, \phi_{\pm, k,l} \neq 0} a_{k,l}.
$$

There are 4 indices $(\pm, k, l)$ where $\phi_{\pm, k,l} = 0 - (\pm, 0, 0)$ and $(\pm, n/2, n/2)$, hence $A = 8$.

Since $\phi_{\pm, k,l} = \phi_{+ k,l}$, it holds that

$$
B = \sum_{\pm, k,l, \phi_{\pm, k,l} \neq 0} a_{k,l} \sin(\phi_{\pm, k,l})
$$

$$
= \sum_{k,l, \phi_{+ k,l} \neq 0} a_{k,l} \sin(\phi_{+ k,l}) - \sum_{k,l, \phi_{- k,l} \neq 0} a_{k,l} \sin(\phi_{- k,l})
$$

$$
= 0.
$$
Finally an approximation of $C$ is

$$C = 2\alpha N \ln(N),$$

where $\alpha \approx 0.32$.

Hence, $\lambda$ is approximated by

$$\lambda = \sqrt{\frac{A}{C}}.$$

This yields to

$$\lambda = \frac{2}{\sqrt{0.33N \ln(N)}},$$

and

$$\lambda' = -\frac{2}{\sqrt{0.33N \ln(N)}} = -\lambda.$$

Now we compute the coefficients $|\langle m | \lambda \rangle|^2$ and $|\langle \lambda | \psi(0) \rangle|^2$.

Supposing $\lambda \neq \phi_{\pm,k,l}$, we obtain

$$\langle \lambda | \psi_{pn,k,l} \rangle = (1 + i\delta_{\pm,k,l}) \langle \psi_{\pm,k,l} | 0 \rangle \langle 0 | \lambda \rangle.$$

We recall that the initial state $\psi(0)$ is the diagonal state, hence $\psi(0) = \psi_{+,0,0}$. Thus

$$\langle \lambda | \psi(0) \rangle = \langle \lambda | \psi_{+,0,0} \rangle = (1 + i\delta_{+,0,0}) \langle \psi_{+,0,0} | 0 \rangle \langle 0 | \lambda \rangle.$$

In order to compute $|\langle 0 | \lambda \rangle|^2$, we look at the constraint

$$\langle \lambda | \lambda \rangle = \langle \lambda | I | \lambda \rangle = \langle \lambda | \sum_{\pm,k,l} |\psi_{\pm,k,l} \rangle \langle \psi_{\pm,k,l} | \lambda \rangle = \sum_{\pm,k,l} |\langle \psi_{\pm,k,l} | \lambda \rangle|^2 = 1.$$

Thus it holds that

$$\sum_{\pm,k,l} |\langle \psi_{\pm,k,l} | \lambda \rangle|^2 = \sum_{\pm,k,l} |1 + i\delta_{\pm,k,l}| \langle \psi_{\pm,k,l} | 0 \rangle \langle 0 | \lambda \rangle|^2 = |\langle 0 | \lambda \rangle|^2 \sum_{\pm,k,l} |1 + i\delta_{\pm,k,l}|^2 = 1.$$  

Now let’s find the value of $|\langle 0 | \lambda \rangle|^2$.

1. $|\langle 0 | \lambda \rangle|^2 = \frac{|\langle 0 | \lambda \rangle|^2}{N} \sum_{\pm,k,l} |1 + i\delta_{\pm,k,l}|^2$

Thus, it holds that

$$|\langle 0 | \lambda \rangle|^2 = \frac{N}{2C}.$$

Now let’s go back to the computation of $|\langle \lambda | \psi(0) \rangle|^2$.

$$|\langle \lambda | \psi(0) \rangle|^2 = |(1 + i\delta_{+,0,0}) \langle \psi_{+,0,0} | 0 \rangle \langle 0 | \lambda \rangle|^2 = \frac{N^2}{2C} \frac{2}{1 - \cos(2\lambda)} \approx \frac{1}{C A^2}.$$

We can compute $c$ knowing $p(0)$.

3. Probability of success and hitting time

Let’s recapitulate here, we have

- $\lambda = \sqrt{\frac{A}{C}} = \frac{2}{\sqrt{\alpha N \ln(N)}}$
- $|\langle m | \lambda \rangle \langle \lambda | \psi(0) \rangle|^2 = \frac{N}{8C} = \frac{1}{16\alpha \ln(N)}$

Now we can use the equation ?? to compute the hitting time and success probability.

We remind that

$$p(t) = 4 \sum_{m \in M} |\langle m | \lambda \rangle \langle \lambda | \psi(0) \rangle|^2 \sin^2(\lambda t + c).$$

In our case, the probability of success $p(t)$ is

$$p(t) = \frac{1}{4\alpha \ln(N)} \sin^2\left(\frac{\lambda t + c}{\sqrt{\alpha N \ln(N)}}\right),$$

where $c$ is a small constant.

We can compute $c$ knowing $p(0)$.

$$c = -\arcsin\left(\sqrt{\frac{4\alpha \ln(N)}{N}}\right).$$

We can now set the optimal success probability $p(t_{opt}) = \frac{1}{\alpha \ln(N)}$ and deduce the hitting time

$$t_{opt} = \frac{\pi}{4} \sqrt{\alpha N \ln(N) + \alpha \ln(N)}.$$
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