# Optimality conditions for spatial search with multiple marked vertices

Mathieu Roget, Hachem Kadri, and Giuseppe Di Molfetta*
*Aix Marseille Univ, Université de Toulon, CNRS, LIS, 13397 Marseille Cedex 20, France*

(Received 1 January 2023; accepted 20 June 2023; published 11 July 2023)

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 searching more than one element, the behavior of the algorithm may be affected by the spatial configuration of the marked elements and even the quantum advantage is no longer guaranteed. Here our main contribution is threefold: (i) we provide sufficient conditions for optimality for a multi-items QWSearch algorithm; (ii) we provide analytical evidence that almost, but not all spatial configurations with multiple marked elements are optimal; and (iii) we numerically show that the computational advantage with respect to the classical counterpart is not always certain and it does depend on the proportion of searched elements over the total number of grid points.

DOI: 10.1103/PhysRevResearch.5.033021

## I. INTRODUCTION

One of the main applications of quantum computing is algorithmic. 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 optimize computing time and quantum resources. However, compared to the thousands of nonquantum 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 problems in quantum computing: *the quantum search* in an unstructured set of $N$ elements. The first algorithm aiming to solve this problem appeared in Grover's [7] work. 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 $O(\sqrt{N})$ 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 speedup 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 speedup. Such quantum advantage has been proven for several generalizations, for instance when the target elements are multiple [12]. However, the situation may be dramatically different for *spatial* searching, where quadratic speedup 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 now involves 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 speedup with 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 (also known as 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 a very different scenario. Such a scenario has been mentioned first by Aaronson and Ambainis [15] and recently observed by Bezerra *et al.* [16], but has never been studied and fully understood. Yet traditionally, it has been assumed that when the number of elements searched is low, the spatial search algorithm is optimal. In this paper, we will prove this assumption false. In fact, we will prove that even

*giuseppe.dimolfetta@lis-lab.fr

when considering only two searched elements, there is always a set of spatial configurations for which the search algorithm is suboptimal. Fortunately, we need not worry because this number is small compared to the number of optimal configurations, for all practical purposes. More specifically, we will show that almost all configurations with two marked elements are optimal [complexity in $O(\sqrt{N}\text{polylog}(N))$], and we will be able to precisely upper bound the number of nonoptimal configurations [complexity in $O(N)$]. As a byproduct of this rigorous result, we will provide a set of sufficient conditions on the searched elements' relative position on the grid to ensure the optimality of the algorithm. Finally, we discuss the results and we provide strong numerical evidence that such nonoptimality issue is not only present when the number of marked elements is two. More generally, the quantum advantage will be shown to not always be guaranteed and also strictly depending on the ratio of marked elements $M/N$, with $M$ the number of the searched elements on the grid.

*Optimality.* In this article, the quantum walk search algorithm we consider is based on an alternated coined quantum walk, as introduced by Di Franco *et al.* [17], defined on a grid of size $\sqrt{N} \times \sqrt{N}$ with $M$ the number of marked elements. We call a configuration for which the QWSearch algorithm solve the searching problem in $O(\sqrt{N/M})$ modulo some $\log(N/M)$ coefficient optimal. These configurations are called optimal because we cannot do better than that for this specific algorithm on a grid. However, in this work, we show that we can surprisingly do worse without having the searching process completely collapsing for $M = 2$.

*Related work.* The search problem for multiple marked elements has been addressed by several authors and in different frameworks. In the discrete-time mathematical framework, Ambainis and Rivosh tackled this problem using a quantum walk-based algorithm and observed for the first time that some specific configurations could lead to a failure while searching [18]. They named this kind of configuration "exceptional configurations." This work was followed by Nahimovs and Rivosh [19], in the framework of the Grover coined QW, where the authors used topological arguments to prove the existence of such configurations for which the search completely fails. Later on, Bezerra *et al.* [16] argued that the relative position of the marked elements might affect the searching behavior. However, the general solution to this problem remained essentially open. In fact, all the above results lack generality and rely on very specific configurations. In particular, most of them qualify this configuration of exceptional. It is important here to distinguish exceptional configurations, for which the searching algorithms fail, from the nonoptimal configurations. For such configurations, there exist solutions to the searching problem, but they are nonoptimal. We aim to investigate such configurations in this article. Multitarget searching has been studied also in the continuous time framework, e.g., by Wong *et al.* [20], who showed how one can search multiple marked vertices on the simplex of complete graphs. They provided numerical evidence that, for some particular configurations of marked elements, the search is affected and might even fail entirely. Moreover, only a few of the aforementioned authors provided analytical solutions. Finally, in all of them the common conjecture is that for a well defined QWSearching algorithm, the search would either be optimal or completely fail for rare exceptional configurations. In the following, we prove the existence of configurations for which the search is working but suboptimal. Moreover, we do not only prove that nonoptimal configurations of two marked elements exist, we also introduce a necessary condition for them to appear and bound their number.

## II. A TWO-DIMENSIONAL, DISCRETE TIME QUANTUM WALK SEARCH (QWSEARCH) ALGORITHM

A discrete time quantum walk on a grid is the quantum analog of a two-dimensional random walk. The quantum walker lives in a composite Hilbert space: The coin state space, encoding the walker direction, and the position state space. The physical space here is a grid of size $\sqrt{N} \times \sqrt{N}$. A generic state of the walker reads as follows:

$$|\psi\rangle = \sum_{v\in\{0,1\}} \sum_{x=0}^{\sqrt{N-1}} \sum_{y=0}^{\sqrt{N-1}} \alpha_{v,x,y}|v, x, y\rangle,$$

where the coin state space is spanned by the $z$ basis $\{|0\rangle, |1\rangle\}$. The walker evolves driven by the usual split-step operator:

$$U = \Sigma_y(C_y \otimes \mathbb{1}_N)\Sigma_x(C_x \otimes \mathbb{1}_N),$$

where $C_y$ and $C_x$ are two noncommutative $U(2)$ operators and the $\Sigma_i$, are coin state dependent shift operators along direction $i = x, y$, defined as follows:

$$\Sigma_i|v\rangle|i\rangle = |v\rangle|i - (-1)^v\rangle.$$

The search algorithm based on the aforementioned quantum walk scheme (QWSearch), for a set of marked vertices $|m\rangle \in \mathcal{M}$, was already considered in, e.g., [21], and it is implemented as follows: (i) Initialize the quantum walker $\psi(0)$ to the equal superposition over all states; when $n$ is a power of two this can be done by applying $n$ single bit Hadamard operation to the ground state $|0\rangle$. (ii) Given a coin oracle $R = \mathbb{1} - 2\sum_{m\in\mathcal{M}} |d, m\rangle\langle d, m|$, where $|d\rangle$ is the diagonal state $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$ in the coin state space, apply the perturbed evolution operator $U' = UR$ for $t_{\text{opt}}$ steps, the hitting time. (iii) Measure the state in the $|v, x, y\rangle$ basis. The success probability of the walker $p(t)$ after $t$ time steps is given by

$$p(t) = \sum_{m\in\mathcal{M}} |\langle d, m|U'^t|\psi(0)\rangle|^2.$$

When searching one marked element, it can be shown that the final complexity is $O(\sqrt{N}\ln^{3/2} N)$, which is quite conventional compared to other quantum walked search algorithms. In the next sections we will investigate what happens when several vertices are marked.

## III. ANALYTICAL RESULTS FOR TWO MARKED VERTICES

Let us now consider the algorithm presented above when there are two marked vertices, $m_0 = (0, 0)$ and $m_1 = (x, y)$. The success probability of the walker $p(t)$ after $t$ time steps is given by

$$p(t) = \sum_{m\in\mathcal{M}} |\langle d, m|U'^{t}|\psi(0)\rangle|^2$$
$$= \sum_{j=0,1} \left|\sum_{\theta} e^{i\theta t}\langle d, m_j|\theta\rangle\langle\theta|\psi(0)\rangle\right|^2,$$

where the operator $U'$ has been diagonalized on its basis. The main aim here is to find the hitting time $t_{\rm opt}$ which maximizes the above probability. Assuming that the search algorithm converges in finite time, one shall expect that the eigenspace of $U'$ be approximately spanned by $\{|\lambda_+\rangle, |\lambda_-\rangle\}$, with $e^{i\lambda_+}$ and $e^{i\lambda_-}$ the two closest eigenvalues to unity:

$$\lambda_+ = \min_{e^{i\theta}\in\sigma}(U'),\ \theta > 0\theta \ \text{ and } \ \lambda_- = \max_{e^{i\theta}\in\sigma}(U'),\ \theta < 0\theta.$$

Thus, let us cast all the negligible contributions as $\epsilon_m$:

$$p(t) = \sum_{j=0,1} |\beta_{+,j}e^{i\lambda_+ t} + \beta_{-,j}e^{i\lambda_- t} + \epsilon_m|^2. \tag{1}$$

To analytically calculate the probability of success, we must therefore obtain an explicit expression of the coefficients $\beta_{i,j} = \langle d, m_j|\lambda_i\rangle\langle\lambda_i|\psi(0)\rangle$. To begin with, let us consider the eigenmodes of the QW operator $|\psi_{\pm k,l}\rangle$ with eigenvalues $e^{i\phi_{\pm k,l}}$. We can point out that $\langle\psi_{\pm k,l}|\lambda_i\rangle$ can be expressed in terms of $\langle d, m_j|\lambda_i\rangle$. In fact,

$$\langle\psi_{\pm k,l}|U'|\lambda_i\rangle$$
$$= e^{i\phi_{\pm k,l}}\langle\psi_{\pm k,l}|\lambda_i\rangle - 2e^{i\phi_{\pm k,l}}\sum_{j=0,1}\langle\psi_{\pm k,l}|d, m_j\rangle\langle d, m_j|\lambda_i\rangle,$$

which leads to

$$\langle\psi_{\pm k,l}|\lambda_i\rangle = \frac{2}{1 - e^{i(\lambda_i - \phi_{\pm k,l})}}\sum_{j=0,1}\langle\psi_{\pm k,l}|d, m_j\rangle\langle d, m_j|\lambda_i\rangle. \tag{2}$$

Moreover, since $\lambda_i$ is close to zero, the prefactor of the sum can be approximated as follows:

$$\frac{2}{1 - e^{i(\lambda_i - \phi_{\pm k,l})}} = 1 + ib^{\lambda}_{\pm k,l},$$

where

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

From Eq. (2) and using the completeness relation, we recover the characteristic equation:

$$\Lambda^{\lambda}\langle d, m_j|\lambda_i\rangle = 0, \tag{3}$$

where the symmetric square matrix $\Lambda$ has elements

$$\Lambda^{\lambda}_{j,j'} = \sum_{a=\pm,k,l} b^{\lambda}_{a,k,l}\langle d, m_j \mid \psi_{a,k,l}\rangle\langle\psi_{a,k,l} \mid d, m_{j'}\rangle.$$

### A. Computation of $\Lambda^{\lambda}$

We will now start computing $\Lambda^{\lambda}$, but, before that, we provide the explicit expressions for the eigenvalues and eigenvectors of $U$:

$$|\psi_{a,k,l}\rangle = |v_{a,k,l}\rangle \otimes \frac{1}{\sqrt{N}}\sum_{j,j'} e^{2i\pi\frac{kj+lj'}{\sqrt{N}}}|j, j'\rangle, \tag{4}$$

$$\phi_{a,k,l} = a\arccos\left(\cos\frac{2\pi k}{\sqrt{N}}\cos\frac{2\pi l}{\sqrt{N}}\right), \tag{5}$$

$$|\langle d \mid v_{a,k,l}\rangle|^2 = \frac{1}{2} - a\frac{1}{4}\frac{\sin\frac{2\pi k}{\sqrt{N}}\sin\frac{2\pi l}{\sqrt{N}}}{\sin\phi_{+,k,l}}\mathbb{1}_{\phi_{a,k,l}\neq 0}. \tag{6}$$

We recall that

$$\Lambda^{\lambda}_{j,j'} = \sum_{a=\pm,k,l} b^{\lambda}_{a,k,l}\langle d, m_j \mid \psi_{a,k,l}\rangle\langle\psi_{a,k,l} \mid d, m_{j'}\rangle.$$

In order to simplify the coefficients of $\Lambda^{\lambda}$, we use the explicit form of $\psi_{a,k,l}$ to show that

$$\langle d, m_j \mid \psi_{a,k,l}\rangle\langle\psi_{a,k,l} \mid d, m_{j'}\rangle$$
$$= \langle d \mid v_{a,k,l}\rangle\langle m_j \mid \psi_{a,k,l}\rangle\langle v_{a,k,l} \mid d\rangle\langle\psi_{a,k,l} \mid m_{j'}\rangle$$
$$= \frac{|\langle d \mid v_{a,k,l}\rangle|^2}{N}\exp^{2i\pi\frac{k(x_j - x_{j'}) + l(y_j - y_{j'})}{\sqrt{N}}},$$

then

$$\langle d, m_j \mid \psi_{a,k,l}\rangle\langle\psi_{a,k,l} \mid d, m_{j'}\rangle$$
$$= \begin{cases}\frac{|\langle d|v_{a,k,l}\rangle|^2}{N} & \text{if } j = j'\\ \frac{|\langle d|v_{a,k,l}\rangle|^2}{N}e^{\pm 2i\pi\frac{kx+ly}{\sqrt{N}}} & \text{otherwise.}\end{cases} \tag{7}$$

The main idea now is to use Eq. (3) to cut the coefficients $\Lambda^{\lambda}_{j,j'}$ into three cases. Let us start for the coefficients $\Lambda^{\lambda}_{j,j}$:

$$N\Lambda^{\lambda}_{j,j} = N\sum_{a=\pm,k,l} b^{\lambda}_{a,k,l}\langle d, m_j \mid \psi_{a,k,l}\rangle\langle\psi_{a,k,l} \mid d, m_j\rangle, \qquad \text{according to Eq. (3)}$$
$$= \sum_{a=\pm,k,l} b^{\lambda}_{a,k,l}|\langle d \mid v_{a,k,l}\rangle|^2, \qquad \text{using Eq. (7)}$$
$$\sim \sum_{\phi_{a,k,l}=0}\frac{2}{\lambda}|\langle d \mid v_{a,k,l}\rangle|^2 - \sum_{\phi_{a,k,l}\neq 0}\frac{(\sin\phi_{a,k,l}) + \lambda}{1 - \cos\phi_{a,k,l}}|\langle d \mid v_{a,k,l}\rangle|^2, \qquad \text{using Eq. (3)}$$
$$= \frac{1}{\lambda}\sum_{\phi_{a,k,l}=0} 1 + \frac{1}{2}\sum_{\phi_{+,k,l}\neq 0}\frac{\sin\frac{2\pi k}{\sqrt{N}}\sin\frac{2\pi l}{\sqrt{N}}}{1 - \cos\frac{2\pi k}{\sqrt{N}}\cos\frac{2\pi l}{\sqrt{N}}} - \lambda\sum_{\phi_{+,k,l}\neq 0}\frac{1}{1 - \cos\frac{2\pi k}{\sqrt{N}}\cos\frac{2\pi l}{\sqrt{N}}}, \qquad \text{using Eq. (4).}$$

First, it is straightforward to prove that there are four possible cases for $\phi_{a,k,l} = 0$, thus $\sum_{\phi_{a,k,l}=0} 1 = 4$. Furthermore, one can show that the second sum $\frac{1}{2}\sum_{\phi_{+,k,l}\neq 0} \frac{\sin\frac{2\pi k}{\sqrt{N}}\sin\frac{2\pi l}{\sqrt{N}}}{1-\cos\frac{2\pi k}{\sqrt{N}}\cos\frac{2\pi l}{\sqrt{N}}} = \frac{1}{2}\sum_{\phi_{k,l}\neq 0} S_{k,l}$ is vanishing, using the symmetry $S_{k,l} = -S_{n-k,l}$. Moreover the last sum can be approximated using integral bounding, resulting in $\sum_{\phi_{+,k,l}\neq 0} \frac{1}{1-\cos\frac{2\pi k}{\sqrt{N}}\cos\frac{2\pi l}{\sqrt{N}}} \sim \frac{1}{\pi} N \ln N$. And finally,

$$\Lambda^{\lambda}_{j,j} \sim \frac{4}{\lambda} - \lambda\frac{N\ln N}{\pi}. \tag{8}$$

Let us now compute the other half of the $\Lambda^{\lambda}$'s coefficients. By using a similar procedure,

$$\begin{aligned} N\Lambda^{\lambda}_{j,j} \sim{}& \frac{1}{\lambda}\sum_{\phi_{a,k,l}=0} e^{\pm 2i\pi\frac{kx+ly}{\sqrt{N}}} \\ &+ \frac{1}{2}\sum_{\phi_{+,k,l}\neq 0} \frac{\sin\frac{2\pi k}{\sqrt{N}}\sin\frac{2\pi l}{\sqrt{N}}}{1-\cos\frac{2\pi k}{\sqrt{N}}\cos\frac{2\pi l}{\sqrt{N}}} e^{\pm 2i\pi\frac{kx+ly}{\sqrt{N}}} \\ &- \lambda\sum_{\phi_{+,k,l}\neq 0} \frac{1}{1-\cos\frac{2\pi k}{\sqrt{N}}\cos\frac{2\pi l}{\sqrt{N}}} e^{\pm 2i\pi\frac{kx+ly}{\sqrt{N}}}. \end{aligned}$$

Now, we can study separately *case i* and *case ii*.

*Case i: $x+y$ odd.* All three above addends are identically vanishing by symmetry. In particular, for each addend $S_{k+\frac{n}{2},l+\frac{n}{2}} = (-1)^{x+y} S_{k,l}$. Consequently,

$$\Lambda^{\lambda}_{j,j'} = 0, \tag{9}$$

with $j \neq j'$ and $x+y$ odd.

*Case ii: $x+y$ even.* The first sum $\sum_{\phi_{a,k,l}=0} e^{\pm 2i\pi\frac{kx+ly}{\sqrt{N}}} = 4$. The other two sums are harder to compute. We can, however, retrieve the expressions of $\mathcal{I}$ and $\mathcal{M}$ by using the symmetry $S_{n-k,n-l} = \overline{S_{k,l}}$. This symmetry implies that the sum is real. We can thus discard the imaginary part. In conclusion,

$$N\Lambda^{\lambda}_{j,j} \sim \frac{4}{\lambda} - \mathcal{I} - \lambda\mathcal{M},$$

where

$$\mathcal{I} = \frac{-1}{2}\sum_{\phi_{+,k,l}\neq 0} \frac{\sin\frac{2\pi k}{\sqrt{N}}\sin\frac{2\pi l}{\sqrt{N}}}{1-\cos\frac{2\pi k}{\sqrt{N}}\cos\frac{2\pi l}{\sqrt{N}}}\cos\left(2\pi\frac{kx+ly}{\sqrt{N}}\right)$$

and

$$\mathcal{M} = \sum_{\phi_{+,k,l}\neq 0} \frac{\cos\left(2\pi\frac{kx+ly}{\sqrt{N}}\right)}{1-\cos\frac{2\pi k}{\sqrt{N}}\cos\frac{2\pi l}{\sqrt{N}}}.$$

To summarize, we have

*Case i.* For $x+y$ odd, then

$$N\Lambda^{\lambda}_{j,j'} \sim \begin{cases} \frac{4}{\lambda} - \lambda\frac{N\ln N}{\pi} & \text{if } j = j' \\ 0 & \text{otherwise,} \end{cases} \tag{10}$$

*Case ii.* For $x+y$ even:

$$N\Lambda^{\lambda}_{j,j'} \sim \begin{cases} \frac{4}{\lambda} - \lambda\frac{N\ln N}{\pi} & \text{if } j = j' \\ \frac{4}{\lambda} - \mathcal{I} - \lambda\mathcal{M} & \text{otherwise.} \end{cases} \tag{11}$$

Now, being the columns of $\Lambda$ are linearly dependent, its determinant is zero. Thus, using Eqs. (10) and (11), we can compute the roots of the equation $\det\Lambda = 0$ which will give us $\lambda_{\pm}$.

### B. Computation of $\lambda_i$ and $|\beta_{i,j}|^2$

We start by using Eqs. (10) and (11) combined with $\det\Lambda^{\lambda} = 0$ [which can be deduced from Eq. (3)] to get $\lambda_{\pm}$. Therefore, we note that $|\langle d, m_0 \mid \lambda_{\pm}\rangle|^2 = |\langle d, m_1 \mid \lambda_{\pm}\rangle|^2$ because of the symmetry of $\Lambda^{\lambda}$. Combining the latter with Eq. (2), we can deduce that

$$\begin{aligned} |\langle\lambda_a|\psi(0)\rangle|^2 &= \left|1 + ib^{\lambda_a}_{+,0,0}\right|^2 \left|\sum_{j=0,1}\langle\psi_{\pm k,l}|d, m_j\rangle\langle d, m_j|\lambda_a\rangle\right|^2 \\ &\sim \frac{8|\langle d, m \mid \lambda\rangle|^2}{N\lambda^2}, \end{aligned} \tag{12}$$

where $|\psi(0)\rangle = |\psi_{+,0,0}\rangle$. One can similarly use Eq. (2) in $\sum_{\pm,k,l}|\langle\psi_{\pm,k,l} \mid \lambda\rangle|^2 = 1$ to show that

$$|\langle d, m \mid \lambda\rangle|^2 \sim \frac{1}{4}\frac{N}{\frac{N\ln N}{\pi} + \mathcal{M}\mathbb{1}_{\{x+y\text{ even}\}}}. \tag{13}$$

Now, using the above result in the expression of $|\langle\lambda_a|\psi(0)\rangle|^2$, we get

$$|\langle\lambda_a|\psi(0)\rangle|^2 \sim \frac{2 + 2.\mathbb{1}_{x+y\text{ even}}}{\lambda^2\left(\frac{N\ln N}{\pi} + \mathcal{M}\mathbb{1}_{\{x+y\text{ even}\}}\right)}. \tag{14}$$

Again, let us consider *case i* and *case ii* separately.

When $x+y$ odd (*case i*), we have

$$\begin{aligned} \det\Lambda^{\lambda} = 0 &\Leftrightarrow \frac{4}{\lambda} - \lambda\frac{N\ln N}{\pi} \sim 0 \\ &\Leftrightarrow \lambda^2 \sim 4\frac{\pi}{N\ln N} \\ &\Leftrightarrow \lambda_{\pm} \sim \pm 2\sqrt{\frac{\pi}{N\ln N}}. \end{aligned} \tag{15}$$

We can now solve explicitly Eqs. (13) and (14) for *Case i* :

$$|\langle d, m \mid \lambda_{\pm}\rangle|^2 \sim \frac{\pi}{4\ln N} \quad\text{and}\quad |\langle\lambda_{\pm}|\psi(0)\rangle|^2 \sim \frac{1}{2}. \tag{16}$$

Notice that the latter expression implies that $\epsilon_m \to 0$. We get $4|\beta_{+,j}|^2 \sim \frac{\pi}{8\ln N}$. The $\lambda_i$ are equal up to a sign, thus Eq. (1) reduces to

$$p(t) \sim 4|\beta_{+,j}|^2\sin^2(\lambda t + \text{cte}) + O(\epsilon_m), \tag{17}$$

where $\lambda = |\lambda_{\pm}|$ and $4|\beta_{+,j}|^2 \sim \frac{\pi}{8\ln N}$, and the hitting time $t_{\text{opt}} \sim \frac{\sqrt{\pi N\ln N}}{4}$. Thus the overall complexity time is $O(\sqrt{N\ln N})$ for a success probability scaling as $O(\ln^{-1}N)$, in line with previous QWSearch for only one element on the grid. We know that this bound is unlikely to be improved, given the strong arguments given by [22–24]. This is not unexpected because the QW operator acts independently onto the sublattice $\mathcal{L}_e = \{(i,j) \mid i+j \text{ even}\}$, with even vertices and the one with odd vertices $\mathcal{L}_o = \{(i,j) \mid i+j \text{ odd}\}$, as we can see in Fig. 1(a). This is due to the bipartite nature of a QW in discrete time makes, so that if the two searched elements are located respectively on white cells and black cells of a chessboard, the QWSearch is running two parallel and independent searches. Now, let us consider $x+y$ even. The determinant of $\Lambda$ reads:

$$\begin{aligned}
\det \Lambda^{\lambda} = 0 &\Leftrightarrow \left(\Lambda^{\lambda}_{0,0}\right)^2 - \left(\Lambda^{\lambda}_{1,0}\right)^2 = 0 && \text{because } \Lambda^{\lambda} \text{ is symmetric}\\
&\Leftrightarrow \left(\Lambda^{\lambda}_{0,0} - \Lambda^{\lambda}_{1,0}\right)\left(\Lambda^{\lambda}_{0,0} + \Lambda^{\lambda}_{1,0}\right) = 0\\
&\Leftrightarrow \left[\mathcal{I} - \lambda\left(\frac{N\ln N}{\pi} - \mathcal{M}\right)\right]\left[\frac{8}{\lambda} - \mathcal{I} - \lambda\left(\frac{N\ln N}{\pi} + \mathcal{M}\right)\right] = 0 && \text{using Eq. (11)}\\
&\Leftrightarrow \lambda_{\pm} \in \left\{\frac{-\mathcal{I} + \sqrt{\mathcal{I}^2 + 32\left(\frac{N\ln N}{\pi} + \mathcal{M}\right)}}{2\left(\frac{N\ln N}{\pi} + \mathcal{M}\right)}, \frac{-\mathcal{I} - \sqrt{\mathcal{I}^2 + 32\left(\frac{N\ln N}{\pi} + \mathcal{M}\right)}}{2\left(\frac{N\ln N}{\pi} + \mathcal{M}\right)}, \frac{\mathcal{I}}{\frac{N\ln N}{\pi} - \mathcal{M}}\right\}.
\end{aligned}$$

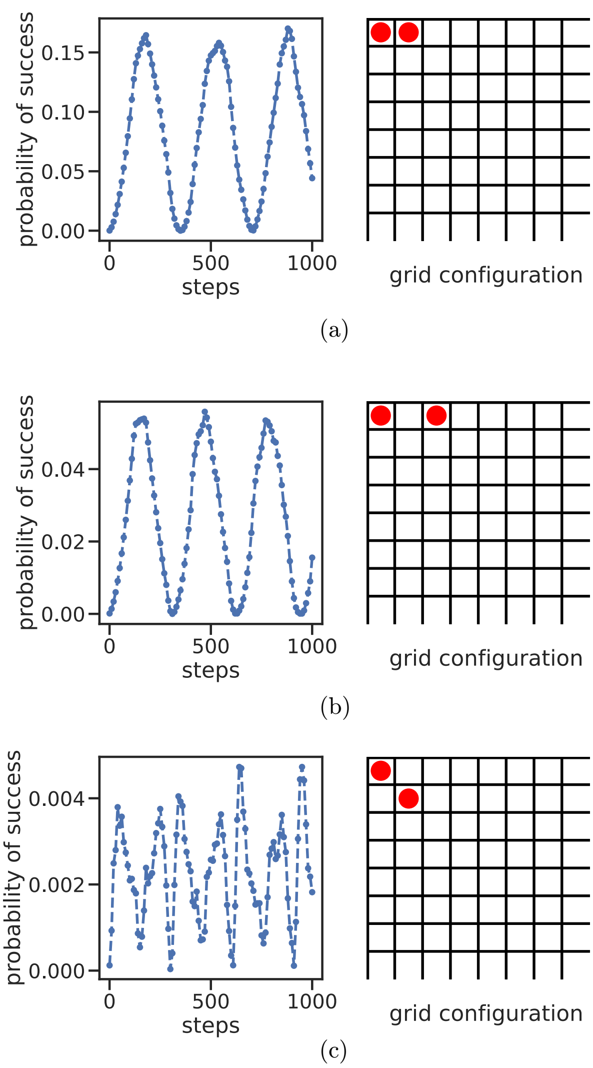


FIG. 1. Three examples of spatial configuration for which the QWSearch algorithms behave differently. (a) Optimal configuration. The searched elements are respectively on the odd and even partition of the grid. The algorithm is always optimal for this configuration. (b) Optimal configuration. Here the optimality of the algorithm is ensured by the condition $\mathcal{I} \ll \mathcal{M} + \frac{N\ln N}{\pi}$, leading to a success probability $O(1/\ln N)$. (c) Nonoptimal configuration. For this configuration the condition $\min(x, n-x)\min(y, n-x) \geqslant n$ does not hold, leading to a success probability $O(1/N)$.

The coefficients $\beta_{i,j} = \langle d, m_j|\lambda_i\rangle\langle\lambda_i|\psi(0)\rangle$ in Eq. (1) read

$$|\beta_{i,j}|^2 \sim \frac{N}{\lambda_i^2\left(\frac{N\ln N}{\pi} + \mathcal{M}\right)^2}.$$

Notice that there are cases where we can manifestly recover optimality. One example is given in Fig. 1(b). Indeed, in the limit

$$\mathcal{I}^2 \ll \mathcal{M} + \frac{N\ln N}{\pi}, \tag{18}$$

the $\lambda_{\pm} \sim \pm\frac{2\sqrt{2}}{\sqrt{\mathcal{M}+\frac{N\ln N}{\pi}}}$, and again the success probability, reduces to Eq. (17) with $\lambda = |\lambda_{\pm}|$ and $|\beta_{+,j}|^2 \sim \frac{N}{8(\frac{N\ln N}{\pi}+\mathcal{M})}$. This result leads to the very same complexity we have in *case i*. It is easy to convince oneself that the condition expressed by Eq. (18) is satisfied in a finite number of cases. In fact, after having computed the sums $\mathcal{I}$, $\mathcal{M}$ and simplified for large $n = \sqrt{N}$, $\mathcal{I} = O(\frac{n^2}{\min(x,n-x)\min(y,n-x)})$ and $0 \leqslant \mathcal{M} \leqslant N\log N$. Then the sufficient condition for a given spatial configuration to be optimal is $\min(x, n-x)\min(y, n-x) = \Omega(n)$. But how many of them do not meet the above condition? It is possible to prove that they are always bounded by $O(n\ln n) = O(\sqrt{N}\ln\sqrt{N})$. Although finite, this number is statistically negligible for large values of $n$. In fact, if one tosses a random configuration, then the probability to find a nonoptimal configuration, such as one in Fig. 1(c), is given by $O(\sqrt{N}\ln\sqrt{N}/N) \xrightarrow{N\to\infty} 0$.

As for *case i*, the latter implies $\epsilon_m \to 0$, meaning that all other eigenvalues of $U'$ can be neglected (including the last solution of $\det\Lambda^{\lambda} = 0$). We finally get $4|\beta_{+,j}|^2 \sim \frac{1}{2}\frac{N}{\frac{N\ln N}{\pi}+\mathcal{M}}$, and using $M \leqslant N\ln N$ we can deduce that the success probability $p_{\rm succ}\,|\beta_{+,j}|^2 = O(\ln^{-1} N)$.

## IV. NUMERICAL RESULTS FOR MORE THAN TWO MARKED VERTICES

Extending the analytical results obtained in this paper to more than two elements is mathematically prohibitive, although feasible in theory. In any case, however, it is possible to show that the number of searched elements, at constant grid size, dramatically affects the advantage over classical

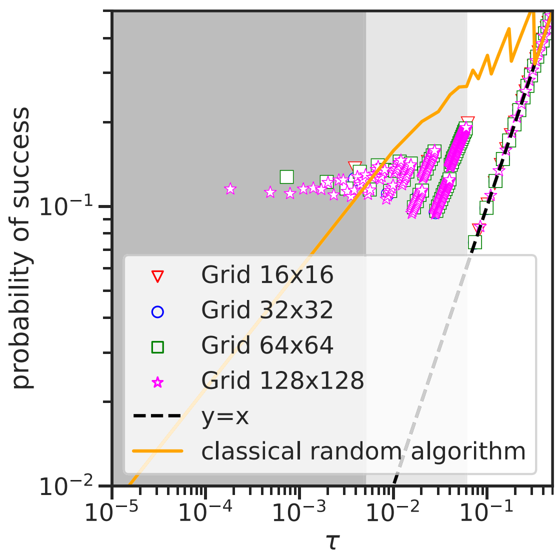


FIG. 2. Average probability of success of QWSearch assuming uniform distribution of the marked elements configuration in function of $\tau = M/N$.

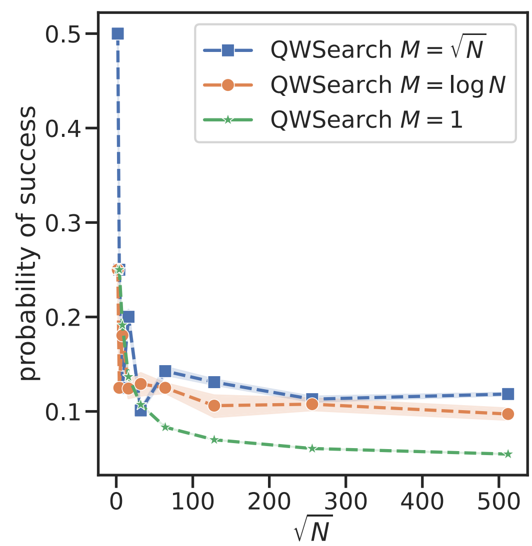


FIG. 3. Average probability of success of the QWSearch algorithm for $M \in \{1, \ln N, \sqrt{N}\}$ in function of $\sqrt{N}$.

search algorithms. The code used to produce the numerical results of this section is available on Github [25]. Let's denote $M$ the number of marked vertices and $\tau = M/N$. In order to search one vertex among the $M$ marked, we may define the following procedure: (i) Shuffle the grid to get a random configuration; (ii) Apply the searching algorithm for $t_{\text{opt}} = \lfloor \sqrt{\pi N/M \ln N/M}/4 \rfloor$ steps; (iii) Measure the final state over the computational basis of the walker. Figure 2 shows the average success probability in function of $\tau$ for several grid sizes. Quite remarkably the success probability does not depend on the grid size. Furthermore, for $\tau$ sufficiently large, the quantum advantage is completely lost and the success probability coincides with the classical one.

To best characterize at what point the advantage is lost, we compare the success probability of our quantum algorithm with respect to a classical algorithm. Our quantum algorithm makes $t_{\text{opt}}$ queries to the oracle. For the same number of queries, we consider a stochastic search algorithm with success probability $p_{cl} = 1 - \frac{N - t_{\text{opt}} M}{NM} \sim 1 - (1 - \tau)^{t_{\text{opt}}}$. The success probability of this algorithm (which depends of $\tau$ only) is displayed in Fig. 2. The critical ratio $\tau_c \approx 0.005$ is the critical ratio upon which the quantum advantage is lost. The darker gray part shows the interval where there is a quantum advantage ($\tau \leqslant \tau_c$) while the lighter gray part shows the interval $\tau_c \leqslant \tau \leqslant 0.1$) in which the QWSearch amplifies the probability of success but is worse than the classical algorithm.

In particular, if the number of marked elements verifies $M = \ln N$ or $M = \sqrt{N}$, then the probability of success of the QWSearch algorithm seems to either tend toward a nonvanishing constant or tend very slowly toward zero. This can be seen in Fig. 3. In particular, the probability of success of the QWSearch algorithm seems to be greater than the classical algorithm for $N$ big enough.

## V. CONCLUSION

We have provided definitive proof that the spatial search algorithm, based on a quantum discrete-time walker, introduced here is not always optimal. We have proved the existence of an upper bound on the number of suboptimal configurations, which remains small for large grid sizes. The proof was obtained in the special case of only two elements searched on the rectangular grid. We have also shown that there is strong numerical evidence that the advantage of the quantum algorithm depends not only on the spatial configuration but also on the ratio of the number of elements searched over the grid size. Such evidence is crucial in order to be able to use the quantum search algorithm correctly, being sure of a quantum advantage, albeit a polynomial one. The sufficiency conditions for optimality are thus relevant for a wide range of applications where the searching algorithm is used as subroutine, from simulation to optimisation and from machine learning to distributed algorithmic.

## ACKNOWLEDGMENTS

This work is supported by the PEPR integrated project EPiQ ANR-22-PETQ-0007; by the ANR JCJC DisQC ANR-22-CE47-0002-01 founded from the French National Research Agency; and the French government under the France 2030 investment plan, as part of the Initiative d'Excellence d'Aix-Marseille Université—A*MIDEX AMX-21-RID-011.

The authors confirm contribution to the paper as follows: Study conception and design: G.D.M. and M.R.; data collection, M.R.; analysis and interpretation of results: G.D.M., M.R., H.K.; draft manuscript preparation: G.D.M. and M.R. All authors reviewed the results and approved the final version of the manuscript.

[1] N. Gisin, G. Ribordy, W. Tittel, and H. Zbinden, Quantum cryptography, Rev. Mod. Phys. **74**, 145 (2002).

[2] J. Biamonte, P. Wittek, N. Pancotti, P. Rebentrost, N. Wiebe, and S. Lloyd, Quantum machine learning, Nature **549**, 195 (2017).

[3] I. M. Georgescu, S. Ashhab, and F. Nori, Quantum simulation, Rev. Mod. Phys. **86**, 153 (2014).

[4] D. Deutsch and R. Jozsa, Rapid solution of problems by quantum computation, Proc. R. Soc. London A **439**, 553 (1992).

[5] P. W. Shor, Algorithms for quantum computation: Discrete logarithms and factoring, in *Proceedings of the 35th Annual Symposium on Foundations of Computer Science* (IEEE, 1994), pp. 124–134.

[6] For a comprehensive catalog of quantum algorithms visit https://quantumalgorithmzoo.org.

[7] L. K. Grover, A fast quantum mechanical algorithm for database search, in *Proceedings of the Twenty-Eighth Annual ACM Symposium on Theory of Computing* (ACM, 1996), pp. 212–219.

[8] C. H. Bennett, E. Bernstein, G. Brassard, and U. Vazirani, Strengths and weaknesses of quantum computing, SIAM J. Comput. **26**, 1510 (1997).

[9] A. Ambainis and R. Špalek, Quantum algorithms for matching and network flows, in *Annual Symposium on Theoretical Aspects of Computer Science* (Springer, 2006), pp. 172–183.

[10] B. Casalé, G. Di Molfetta, H. Kadri, and L. Ralaivola, Quantum bandits, Quant. Mach. Intell. **2**, 11 (2020).

[11] A. Montanaro, Quantum algorithms: An overview, npj Quantum Inf. **2**, 15023 (2016).

[12] M. Boyer, G. Brassard, P. Høyer, and A. Tapp, Tight bounds on quantum searching, Fortschr. Phys. **46**, 493 (1998).

[13] A. M. Childs and J. Goldstone, Spatial search by quantum walk, Phys. Rev. A **70**, 022314 (2004).

[14] S. Chakraborty, L. Novo, A. Ambainis, and Y. Omar, Spatial Search by Quantum Walk is Optimal for Almost all Graphs, Phys. Rev. Lett. **116**, 100501 (2016).

[15] S. Aaronson and A. Ambainis, Quantum search of spatial regions, in *Proceedings of the 44th Annual IEEE Symposium on Foundations of Computer Science* (IEEE, 2003), pp. 200–209.

[16] G. Bezerra, P. Lugão, and R. Portugal, Quantum-walk-based search algorithms with multiple marked vertices, Phys. Rev. A **103**, 062202 (2021).

[17] C. Di Franco, M. Mc Gettrick, T. Machida, and T. Busch, Alternate two-dimensional quantum walk with a single-qubit coin, Phys. Rev. A **84**, 042337 (2011).

[18] A. Ambainis and A. Rivosh, *Quantum Walks with Multiple or Moving Marked Locations*, Vol. 4910 of Lecture Notes in Computer Science (Springer, Berlin, Heidelberg, 2008), pp. 485–496.

[19] N. Nahimovs and A. Rivosh, Exceptional configurations of quantum walks with Grover's coin, arXiv:1509.06862 [quant-ph].

[20] T. G. Wong, Spatial search by continuous-time quantum walk with multiple marked vertices, Quant. Info. Proc. **15**, 1411 (2016).

[21] M. Roget, S. Guillet, P. Arrighi, and G. Di Molfetta, Grover Search as a Naturally Occurring Phenomenon, Phys. Rev. Lett. **124**, 180501 (2020).

[22] F. Magniez, A. Nayak, P. C. Richter, and M. Santha, On the hitting times of quantum versus random walks, Algorithmica **63**, 91 (2012).

[23] A. Patel and M. A. Rahaman, Search on a hypercubic lattice using a quantum random walk. I. $d > 2$, Phys. Rev. A **82**, 032330 (2010).

[24] M. Santha, Quantum walk based search algorithms, in *Proceedings of the International Conference on Theory and Applications of Models of Computation* (Springer, 2008), pp. 31–46.

[25] https://github.com/mroget/Paper-code-Optimality-conditions-for-spatial-search-with-multiple-marked-vertices.