*Math. Struct. in Comp. Science* (2010), *vol.* 20, *pp.* 999–1009. 
doi:10.1017/S0960129510000332

# Spatial search on a honeycomb network

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*Received 16 June 2001; revised 8 October 2002*

The spatial search problem consists of minimising the number of steps required to find a given site in a network under the restriction that only oracle queries or translations to neighbouring sites are allowed. We propose a quantum algorithm for the spatial search problem on a honeycomb lattice with $N$ sites and torus-like boundary conditions. The search algorithm is based on a modified quantum walk on an hexagonal lattice and the general framework proposed by Ambainis, Kempe and Rivosh (Ambainis *et al.* 2005) is employed to show that the time complexity of this quantum search algorithm is $O(\sqrt{N \log N})$.

## 1. Introduction

Quantum Walks (QW) are useful tools for generating new quantum algorithms (Ambainis 2004; Shenvi *et al.* 2003; Ambainis *et al.* 2005). For example, the optimal algorithm for solving the element distinctness problem, which aims to determine whether a set has repeated elements or not, is based on QWs (Ambainis 2004). An optimal search algorithm equivalent to Grover's celebrated algorithm (Grover 1996) uses a modified QW on an $n$-dimensional hypercube to find an element among $N$ sites after $O(\sqrt{N})$ steps (Shenvi *et al.* 2003). Although the QW is a unitary (that is, invertible) process, it is often introduced as the quantum analogue of a random walk or, more generally, of a Markov process. There are two versions of QWs: discrete-time (Aharonov *et al.* 1993) and continuous-time (Fahri and Gutmann 1998) walks. The first uses an auxiliary Hilbert space, which plays the role of a quantum 'coin' whose states determine the directions of motion. Even though both types of QW's have similar dynamics, they are not equivalent. For instance, the optimal algorithm for spatial search in two-dimensional grids using the continuous-time version has no advantage over the classical algorithm in terms of time complexity (Childs and Goldstone 2004), while the algorithm based on the discrete-time version has an almost quadratic improvement (Tulsi 2008).

Grover's algorithm applies to non-ordered databases, where there is no notion of distance between two elements. However, when storing information in physical memory, a given item is stored at a specific location. This poses an interesting alternative version of searching, called spatial search, as the problem of finding a marked location in a

rigid structure using only local operations: in one time step one can either query an oracle for the given site or move to a neighbouring site. Benioff addressed this problem on a two-dimensional square lattice with $N$ points (Benioff 2002). He was the first to point out that a straightforward application of Grover's algorithm with the spatial search constraint requires $\Omega(N)$ steps with no improvement over classical algorithms in terms of time complexity. Aaronson and Ambainis have developed a quantum algorithm for this problem with time complexity $O(\sqrt{N}\log^2 N)$ (Aaronson *et al.* 2003). Ambainis, Kempe and Rivosh (AKR) have proposed a QW-based algorithm that improves the time complexity to $O(\sqrt{N}\log N)$ (Ambainis *et al.* 2005). Recently, Tulsi has proposed an improved version of the AKR spatial search algorithm for two-dimensional square lattices with a time complexity of $O(\sqrt{N\log N})$ (Tulsi 2008). It is an open problem whether the lower bound $\Omega(\sqrt{N})$ can be achieved for the spatial search on two-dimensional lattices (Bennet *et al.* 1997). AKR have proposed a generalised framework for QW-based algorithms on lattices of arbitrary structure in which the time complexity of the algorithm may be obtained from the eigenvalue spectrum of the QW evolution operator. Following AKR, we shall refer to this formalism as the *abstract search framework*.

In this paper, we provide a new QW-based algorithm that solves the spatial search problem in a hexagonal (honeycomb) network in $O(\sqrt{N\log N})$ steps. The time complexity is analysed using the abstract search framework just discussed. The hexagonal network has received attention from condensed matter physicists for many years due to its role in the band theory of graphite (Wallace 1947). More recently, the development of graphenes (two-dimensional hexagonal arrays of Carbon atoms) and their possible uses in quantum computation (Van den Nest *et al.* 2006) have renewed the interest in these networks (Geim *et al.* 2007).

The paper is organised as follows. In Section 2 we discuss the implementation of a quantum walk on a periodic hexagonal network and obtain the evolution operator in the Fourier-transformed space. In Section 3 we summarise the abstract search framework and use it to evaluate the time complexity of the search algorithm on a hexagonal lattice. In Section 4 we present our conclusions.

## 2. QW on the hexagonal network

The Hilbert space of a QW, $\mathscr{H} = \mathscr{H}_C \otimes \mathscr{H}_P$ is composed of a coin, $\mathscr{H}_C$, and a position subspace, $\mathscr{H}_P$. The evolution operator is of the form $U = S \cdot (C \otimes I)$ where $C$ is a unitary operation in $\mathscr{H}_C$, $I$ is the identity in $\mathscr{H}_P$ and $S$, a shift operation in $\mathscr{H}$, performs a conditional one-step displacement as determined by the current coin state. The main challenge in obtaining the time complexity of a QW-based algorithm on a honeycomb lattice is the calculation of the spectral decomposition of the evolution operator $U$ of the underlying QW. The abstract search framework is based on a modified evolution operator $U' = S \cdot C'$, obtained from the standard quantum walk operator $U$ by replacing the coin operation $C$ with a new unitary operation $C'$ that is not restricted to $\mathscr{H}_C$ and acts differently on the searched vertex. Ambainis and coworkers have shown that the time complexity of the spatial search algorithm can be obtained from the spectral

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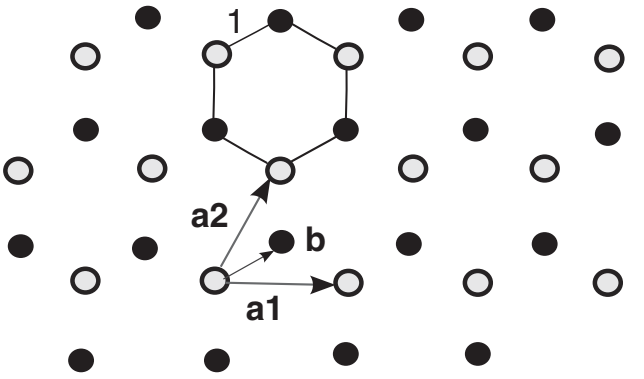


Fig. 1. Elementary vectors for the honeycomb network. The white sites form a lattice and black sites form the associated basis.

decomposition of the evolution operator $U$ of the unmodified QW (Ambainis *et al.* 2005), which is usually simpler than that of $U'$.

In regular networks, the use of the Fourier transform on the spatial coordinates considerably simplifies the expressions for the eigenvalues and eigenvectors. It is known that a Bravais lattice has an associated reciprocal lattice (Kittel 1995) and that this provides a systematic way of obtaining the Fourier transform. The honeycomb network is not a Bravais lattice, but this can be circumvented by splitting the vertices into two sets with $N/2$ sites each (the lattice and basis sets) and encoding the which-set information on an auxiliary one-qubit state. In Figure 1, we distinguish between the $N/2$ lattice sites (gray) and the $N/2$ basis sites (black) using a colour code.

Let us consider the distance between two adjacent sites of the hexagonal network as the unit distance. Then, the vectors $\mathbf{a_1}$ and $\mathbf{a_2}$ connecting two neighbouring lattice sites (see Figure 1) have norm $\sqrt{3}$ and span an angle of $60^o$. The unit vector $\mathbf{b}$ that locates the basis site adjacent to a given lattice site is given by $\mathbf{b} = \frac{1}{3}(\mathbf{a_1} + \mathbf{a_2})$. An arbitrary lattice point may be addressed by a vector with integer components

$$\mathbf{r} = n_1\mathbf{a_1} + n_2\mathbf{a_2} \tag{1}$$

and each lattice point has an associated basis point at $\mathbf{r} + \mathbf{b}$. We assume periodicity in both directions (von Karmann boundary conditions), so that $n_1, n_2 \in [0, m-1]$. For simplicity, we consider a number of sites $N$ such that $N = 2m^2$, for some integer $m$. Thus, for an $N$-element network, we have $N/2$ kets $|n_1, n_2\rangle$ spanning the position subspace associated with the lattice. The $N/2$ basis sites are accounted for by introducing an auxiliary qubit, $\{|0\rangle, |1\rangle\}$, which is zero for a lattice site and 1 for a basis site. Thus, we write $|0; n_1, n_2\rangle \equiv |0\rangle \otimes |n_1, n_2\rangle$ for a state associated with a lattice site and $|1; n_1, n_2\rangle$ for the state associated with the corresponding basis site. The $N$-dimensional lattice subspace $\mathscr{H}_P$ is spanned by kets $\{|s; n_1, n_1\rangle\}$ with $s = 0, 1$.

At a given site there are three possible directions of motion, and we label each of them with an integer index $j = 0, 1, 2$ so that the direction of motion is encoded in a three-dimensional 'coin' subspace $\mathscr{H}_C$ spanned by $\{|0\rangle, |1\rangle, |2\rangle\}$. The full $3N$-dimensional

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Hilbert space is $\mathscr{H} = \mathscr{H}_C \otimes \mathscr{H}_P$ and the basis states $|j;s;n_1,n_2\rangle$ form an orthonormal set. In this basis, a generic state $|\Psi\rangle \in \mathscr{H}$ is expressed as

$$|\Psi\rangle = \sum_{j;n_1,n_2} a_{j,n_1,n_2}|j;0;n_1,n_2\rangle + b_{j,n_1,n_2}|j;1;n_1,n_2\rangle \tag{2}$$

where the complex coefficients $a_{j,n_1,n_2}$ $\left(b_{j,n_1,n_2}\right)$ are the lattice (basis) components and the normalisation condition $\langle\Psi|\Psi\rangle = 1$ is assumed. A step in any direction from a lattice (basis) point leads to a basis (lattice) point according to the propagation rule

$$|j;s;n_1,n_2\rangle \rightarrow |j;\, s\oplus 1;\, n_1-(-1)^s\alpha_j,\, n_2-(-1)^s\beta_j\rangle \tag{3}$$

where $\oplus$ is the binary sum and $\hat{\mathbf{v}}_j = (\alpha_j,\beta_j)$ are the directional vectors

$$\begin{aligned}\hat{\mathbf{v}}_0 &= (0,0)\\ \hat{\mathbf{v}}_1 &= (1,0)\\ \hat{\mathbf{v}}_2 &= (0,1).\end{aligned} \tag{4}$$

This conditional displacement is implemented using a shift operator

$$S = \sum_{j,\,s,\,\hat{\mathbf{n}}} |j,s\oplus 1,\hat{\mathbf{n}}-(-1)^s\,\hat{\mathbf{v}}_j\rangle\langle j,s,\hat{\mathbf{n}}| \tag{5}$$

where we have introduced the shorthand notation $\hat{\boldsymbol{n}}$ for $(n_1,n_2)$ and the sum modulo $m$ is understood for these components. The evolution operator of a quantum walk on the hexagonal network is then

$$U = S\cdot(G_3\otimes I_P) \tag{6}$$

where $I_P$ is the identity in $\mathscr{H}_P$. The three-dimensional Grover operation $G_3$ acts in $\mathscr{H}_C$ and, in the representation stated above, is given by

$$G_3 = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2\\ 2 & -1 & 2\\ 2 & 2 & -1\end{pmatrix}. \tag{7}$$

After $t$ iterations, an initial state $|\Psi_0\rangle$ evolves to $|\Psi_t\rangle = U^t|\Psi_0\rangle$. Note that $U$ is a real operator, as required by the abstract search formalism (Ambainis *et al.* 2005).

For single-step displacements, the spatial part of the evolution operator is diagonal in the Fourier representation, so let us now consider the Fourier transform in $\mathscr{H}_P$. The lattice reciprocal (Kittel 1995) to the one defined by the vectors $\{\mathbf{a_1},\mathbf{a_2}\}$ is formed by vectors $\{\mathbf{g_1},\mathbf{g_2}\}$, which satisfy

$$\begin{aligned}\mathbf{g}_1\cdot\mathbf{a}_1 &= \mathbf{g}_2\cdot\mathbf{a}_2 = 2\pi/m,\\ \mathbf{g}_1\cdot\mathbf{a}_2 &= \mathbf{g}_2\cdot\mathbf{a}_1 = 0.\end{aligned} \tag{8}$$

A point of the reciprocal lattice is located through a vector $\mathbf{k} = k_1\mathbf{g_1} + k_2\mathbf{g_2}$ for integers $k_1,k_2 \in [0,m-1]$. We shall use the shorthand notation $\hat{\mathbf{k}}$ for the two-component vector $(k_1,k_2)$.

The coin components of $|\Psi\rangle$ play no essential role in the following, so we will omit the coin dependence for the moment. So a state $|\Psi\rangle$ can be expressed in either the position

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representation or in the wavenumber representation as

$$|\Psi\rangle = \sum_{\hat{\mathbf{n}}} \left(a_{\hat{n}}|0;\hat{\mathbf{n}}\rangle + b_{\hat{n}}|1;\hat{\mathbf{n}}\rangle\right) = \sum_{\hat{\mathbf{k}}} \left(f_{\hat{k}}|0;\hat{\mathbf{k}}\rangle + g_{\hat{k}}|1;\hat{\mathbf{k}}\rangle\right). \tag{9}$$

The $N$ states $|s;\hat{\mathbf{k}}\rangle$ are related to the position representation by the Fourier transform

$$|s;\hat{\mathbf{k}}\rangle = \sqrt{\frac{2}{N}} \sum_{\hat{\mathbf{n}}} e^{-i\mathbf{k}\cdot\mathbf{r}}|s,\hat{\mathbf{n}}\rangle \tag{10}$$

$$|s;\hat{\mathbf{n}}\rangle = \sqrt{\frac{2}{N}} \sum_{\hat{\mathbf{k}}} e^{i\mathbf{k}\cdot\mathbf{r}}|s,\hat{\mathbf{k}}\rangle. \tag{11}$$

These states satisfy $\langle s,\hat{\mathbf{k}}|s',\hat{\mathbf{n}}\rangle = \sqrt{\frac{2}{N}}\, e^{i\mathbf{k}\cdot\mathbf{r}}\, \delta_{s,s'}$, so Fourier transformed kets of lattice (basis) states are orthogonal to basis (lattice) kets.

Taking into account the coin dependence and using the above relations, the action of the shift operator, Equation (5), on $\mathbf{k}$-space is

$$S|j;s;\hat{\mathbf{k}}\rangle = \omega^{-(-1)^s\hat{\mathbf{k}}\cdot\hat{\mathbf{v}}_j}\,|j;s\oplus 1;\hat{\mathbf{k}}\rangle, \tag{12}$$

where $\omega \equiv \exp(2\pi i/m)$ and the directional vectors $\hat{\mathbf{v}}_j$ were defined in Equation (4). Notice that $S$ is diagonal in $k$-space and connects lattice points with basis points as expected. This fact effectively reduces the problem to a six-dimensional subspace $\mathscr{L}_{\mathbf{k}}$ spanned by the kets $\{|j;s\rangle\}$. Since $\hat{\mathbf{k}}$ takes $N/2$ values, the Hilbert space is now decomposed in this subspace and the one spanned by the $|\hat{\mathbf{k}}\rangle$ states, with a dimensional count $6 \times N/2 = 3N$. In this six-dimensional subspace, in the representation stated above, the reduced evolution operator $U_{\mathbf{k}}$ has the explicit form

$$U_{\mathbf{k}} = \begin{pmatrix} 0 & -\frac{1}{3} & 0 & \frac{2}{3} & 0 & \frac{2}{3} \\ -\frac{1}{3} & 0 & \frac{2}{3} & 0 & \frac{2}{3} & 0 \\ 0 & \frac{2}{3}\,\omega^{k_1} & 0 & -\frac{1}{3}\,\omega^{k_1} & 0 & \frac{2}{3}\,\omega^{k_1} \\ \frac{2}{3}\,\omega^{-k_1} & 0 & -\frac{1}{3}\,\omega^{-k_1} & 0 & \frac{2}{3}\,\omega^{-k_1} & 0 \\ 0 & \frac{2}{3}\,\omega^{k_2} & 0 & \frac{2}{3}\,\omega^{k_2} & 0 & -\frac{1}{3}\,\omega^{k_2} \\ \frac{2}{3}\,\omega^{-k_2} & 0 & \frac{2}{3}\,\omega^{-k_2} & 0 & -\frac{1}{3}\,\omega^{-k_2} & 0 \end{pmatrix} \tag{13}$$

Its characteristic polynomial factors as

$$P(\lambda) = (\lambda - 1)(\lambda + 1)(\lambda^4 - 2\cos(2\theta_k)\,\lambda^2 + 1), \tag{14}$$

where the angle $\theta_k \in [0, \frac{\pi}{2}]$ is defined by

$$\cos(2\theta_k) \equiv \frac{4}{9}\left(\cos\tilde{k}_1 + \cos\tilde{k}_2 + \cos\left(\tilde{k}_1 - \tilde{k}_2\right)\right) - \frac{1}{3}, \tag{15}$$

and $\tilde{k}_i \equiv 2\pi k_i/m$ for $i = 1, 2$. The six eigenvalues of $U_{\mathbf{k}}$ are $\pm 1$ and $\pm e^{\pm i\theta_k}$.

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## 3. Time complexity of the search algorithm

The abstract search formalism described in Ambainis *et al.* (2005) provides a way to implement a spatial search algorithm on a network where a QW has been properly defined. A convenient summary of the abstract search formalism can be found in Tulsi (2008).

Assume that the search is for a single site $\mathbf{r} = \mathbf{r_0}$ in a periodic hexagonal (honeycomb) network with $N$ sites. The effective target state in $\mathscr{H}$ is $|t\rangle \equiv |u\rangle \otimes |\mathbf{r_0}\rangle$ where $|u\rangle = (1/\sqrt{6})\sum_{j,s}|j,s\rangle$ is the uniform superposition in $\mathscr{L}_{\mathbf{k}}$.

The generalised search algorithm iterates the unitary operator

$$U' = U \cdot R_t, \tag{16}$$

where $U$ is the unperturbed quantum walk operator defined in Equation (6) and $R_t \equiv I_{3N} - 2|t\rangle\langle t|$. In the introduction we mentioned that a generalised search is implemented with a modified quantum walk operator of the form $U' = S \cdot C'$, where $C'$ is a unitary coin operation that acts differently on the searched site, that is,

$$C' = C \otimes (I_P - |\mathbf{r_0}\rangle\langle\mathbf{r_0}|) + C_1 \otimes |\mathbf{r_0}\rangle\langle\mathbf{r_0}|.$$

Both forms for $U'$ are equivalent, provided the Grover coin $C = G_3$ is used and the usual choice of $C_1 = -I_C$ is made for the coin operation on a searched site.

The initial state for the algorithm is the uniform superposition in $\mathscr{H}$,

$$|\Phi_0\rangle = |u\rangle \otimes |u_P\rangle = \frac{1}{\sqrt{3N}} \sum_{j,s,\hat{\mathbf{n}}} |j;s;\hat{\mathbf{n}}\rangle, \tag{17}$$

where

$$|u_P\rangle \equiv \sqrt{\frac{2}{N}} \sum_{\hat{\mathbf{n}}} |\hat{\mathbf{n}}\rangle$$

is the uniform superposition in position space. Apart from a phase shift, the operator $R_t$ implements a reflection about the effective target $|t\rangle$ and a single application of $R_t$ on the uniform superposition 'marks' the searched state by changing its relative phase in a similar way to Grover's search algorithm (Grover 1996).

As mentioned previously, Ambainis *et al.* proved the remarkable result that the time complexity of the abstract search algorithm depends on the eigenproblem of $U$ alone (Ambainis *et al.* 2005). They showed that, after $T = O(1/\alpha)$ iterations of $U_A$, the initial state evolves to a final state $|\Phi_f\rangle = U_A^T|\Phi_0\rangle$, which has an increased overlap $|\langle\Phi_f|t\rangle|$ with the effective searched state $|t\rangle$. Detailed expressions for the dependence of $\alpha$ and $\langle\Phi_f|t\rangle$ on the eigenvalues and eigenvectors of $U$ are given below. The unperturbed operator $U$ must satisfy two conditions:

(i) $U$ must be a real operator.
(ii) The uniform superposition state $|\Phi_0\rangle$ must be a non-degenerate eigenstate of $U$ with eigenvalue 1.

Both conditions are met by the quantum walk operator $U$ defined in Equation (6) since $G_3$ is real and $(G_3 \otimes I_2)|u\rangle = |u\rangle$.

We follow the notation of Tulsi (2008) to describe the eigenproblem for $U$. The eigenvectors associated with the $-1$ eigenvalue, which may be $M$-degenerate, are labelled

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as $|\Phi_i\rangle$ for $i = 1 \ldots M$. We write $|\Phi_\ell^\pm\rangle$ for the eigenvectors associated with all other eigenvalues distinct from $\pm 1$. The eigenvectors may be chosen so that the amplitudes on $|t\rangle$ on the proper basis of $U$ are real. The effective target state may then be expanded with real coefficients as

$$|t\rangle = a_0|\Phi_0\rangle + \sum_\ell a_\ell(|\Phi_\ell^+ + \Phi_\ell^-\rangle) + \sum_{i=1}^{M} a_i|\Phi_i\rangle, \tag{18}$$

where the index $\ell$ runs over all pairs of conjugate eigenvectors with eigenvalues distinct from $\pm 1$. These amplitudes $(a_0, a_\ell, a_i)$, together with the angles $\theta_k$ defined by Equation (15), determine the time complexity of the abstract search algorithm (Ambainis *et al.* 2005; Tulsi 2008). The rotation angle towards the searched element, which results from a single application of $U'$, is

$$\alpha = O\left(a_0\left[\sum_\ell \frac{a_\ell^2}{1-\cos\theta_\ell} + \frac{1}{4}\sum_{i=1}^{M} a_i^2\right]^{-\frac{1}{2}}\right). \tag{19}$$

After $T = \pi/2\alpha$ iterations, the overlap with the searched state is

$$|\langle t|\alpha^+\rangle| = O\left(\min\left[\left(\sum_\ell a_\ell^2 \cot^2\frac{\theta_\ell}{4}\right)^{-\frac{1}{2}}, 1\right]\right). \tag{20}$$

In both expressions, the sums $\sum_\ell$ run over the eigenvalues distinct from $\pm 1$.

The (unnormalised) eigenvectors $|v_{\mathbf{k}}^\pm\rangle$ associated with the eigenvalues $\pm 1$ are

$$|v_{\mathbf{k}}^\pm\rangle \propto \begin{pmatrix} \pm(\omega^{k_1} - \omega^{k_2}) \\ \omega^{k_2} - \omega^{k_1} \\ \pm\omega^{k_1}\left(\omega^{k_2} - 1\right) \\ 1 - \omega^{k_2} \\ \pm\omega^{k_2}\left(1 - \omega^{k_1}\right) \\ \omega^{k_1} - 1 \end{pmatrix} \tag{21}$$

except for $k_1 = k_2 = 0$. Note that the projection of the effective target state $|t\rangle$ on $\mathscr{L}_{\mathbf{k}}$ is the uniform state $|u\rangle$ and $\langle u|v_{\mathbf{k}}^\pm\rangle = 0$, unless $k_1 = k_2 = 0$. In this degenerate case, the eigenvalues are $\pm 1$ and $|u\rangle$ itself is an eigenvector of $U_{\mathbf{k}}$ with eigenvalue $+1$. All the other eigenvectors are orthogonal to $|u\rangle$ so, for all $\mathbf{k}$,

$$\langle u|v_{\mathbf{k}}^+\rangle = \delta_{\mathbf{k},\mathbf{0}} \quad \text{and} \quad \langle u|v_{\mathbf{k}}^-\rangle = 0 \tag{22}$$

so that $a_0 = \sqrt{2/N}$ and the terms corresponding to the eigenvalue $-1$ do not contribute in Equation (18). We write the eigenvectors associated with the other eigenvalues $\pm e^{\pm i\theta_k}$

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as $|\pm v_{\mathbf{k}}^{(\pm\theta_k)}\rangle$. Equation (18) for the effective target state then reduces to

$$|t\rangle = \sqrt{\frac{2}{N}}|u, u_P\rangle + \sqrt{\frac{2}{N}}\sum_{\mathbf{k}\neq\mathbf{0}}\Big[a_{\mathbf{k}}^{+}\left(|+v_{\mathbf{k}}^{(\theta_k)}\rangle + |+v_{\mathbf{k}}^{(-\theta_k)}\rangle\right) + a_{\mathbf{k}}^{-}\left(|-v_{\mathbf{k}}^{(\theta_k)}\rangle + |-v_{\mathbf{k}}^{(-\theta_k)}\rangle\right)\Big]\otimes|\mathbf{k}\rangle, \quad (23)$$

with the real amplitudes

$$a_{\mathbf{k}}^{\pm} = \frac{1}{2}\sqrt{1 \pm \frac{1+\cos\tilde{k}_1+\cos\tilde{k}_2}{3\cos\theta_k}}. \quad (24)$$

Even though we do not have analytical expressions for all the eigenvectors of $U$, a knowledge of the coefficients $a_{\mathbf{k}}^{\pm}$ allows us to evaluate the time complexity of the search algorithm.

For the quantum walk on a honeycomb, Equation (19) leads to

$$\frac{1}{\alpha} = O\left(\sqrt{\sum_{\mathbf{k}\neq\mathbf{0}}\frac{(a_{\mathbf{k}}^{+})^2}{1-\cos\theta_k} + \frac{(a_{\mathbf{k}}^{-})^2}{1+\cos\theta_k}}\right) \equiv O\left(\sqrt{A(N)}\right). \quad (25)$$

We now concentrate on the $N$-dependence, for $N \gg 1$, of the argument $A(N)$ of the above square root. Using Equation (24), and after some manipulation, we obtain

$$A = \frac{1}{6}\sum_{\mathbf{k}\neq 0}\frac{4+\cos\tilde{k}_1+\cos\tilde{k}_2}{\sin^2\theta_k} \approx \frac{N}{48}\frac{1}{(\pi-\varepsilon)^2}\iint_{\varepsilon}^{2\pi-\varepsilon} d\tilde{k}_2 d\tilde{k}_1 \frac{4+\cos\tilde{k}_1+\cos\tilde{k}_2}{\sin^2\theta_k} \quad (26)$$

where we have used

$$\sin^2\theta_k = \frac{2}{3} - \frac{2}{9}\left(\cos\tilde{k}_1+\cos\tilde{k}_2+\cos(\tilde{k}_1-\tilde{k}_2)\right)$$

and approximated the sum by an integral in the usual form,

$$\sum_{\mathbf{k}\neq 0} \to \frac{N}{8}\frac{1}{(\pi-\varepsilon)^2}\iint_{\varepsilon}^{2\pi-\varepsilon} d\tilde{k}_1 d\tilde{k}_2$$

with

$$\varepsilon = 2\pi\sqrt{2/N}.$$

For $N \gg 1$ (or $\varepsilon \ll 1$), the $N$-dependence of $A$ is

$$A(N) \simeq \frac{3N}{32}\frac{1}{\pi^2}\int_{\varepsilon}^{2\pi-\varepsilon} d\tilde{k}_2 \int_{\varepsilon}^{2\pi-\varepsilon}\frac{d\tilde{k}_1}{\tilde{k}_1^2+\tilde{k}_2^2-\tilde{k}_1\tilde{k}_2} \sim N\log\left(\frac{2\pi}{\varepsilon}\right) \sim N\log N.$$

So $1/\alpha = O(\sqrt{N\log N})$ iterations of $U'$ are required to reach the final state $|\Phi_f\rangle$.

Using Equation (20), we find that the inverse of the overlap between the final state and the target $|t\rangle$ is

$$|\langle t|\Phi_f\rangle|^{-2} = O\left(\frac{2}{N}\sum_{\mathbf{k}\neq 0}\left[\left(a_k^{+}\right)^2 + \left(a_k^{-}\right)^2\right]\cot^2\left(\theta_k/4\right)\right) \equiv O\left(B(N)\right). \quad (27)$$

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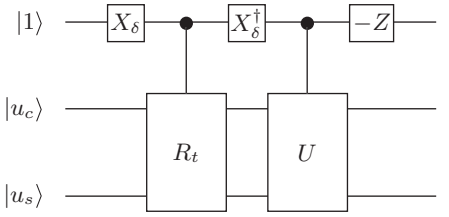


Fig. 2. Tulsi's circuit diagram for the one-step evolution operator of the quantum walk search algorithm.

Using Equation (24) and for $N \gg 1$, the $N$-dependence of $B(N)$ is

$$B(N) \simeq \frac{1}{N}\sum_{\mathbf{k}\neq 0}\cot^2\left(\theta_k/4\right) \simeq \frac{1}{8(\pi-\varepsilon)^2}\iint_{\varepsilon}^{2\pi-\varepsilon} d\tilde{k}_2 d\tilde{k}_1 \cot^2\left(\frac{\theta_k}{4}\right) \sim \log N, \tag{28}$$

where the divergence comes, as before, from the $\sin^{-2}\theta_k$ term. Hence

$$\frac{1}{|\langle t|\Phi_f\rangle|^2} = O\left(\log N\right). \tag{29}$$

The analysis of the time complexity of the algorithm is as follows. After $1/\alpha = O(\sqrt{N\log N})$ iterations of $U'$, the algorithm reaches the final state $|\Phi_f\rangle$ with probability $p = |\langle t|\Phi_f\rangle|^2$. The method known as amplitude amplification (Brassard *et al.* 2002) states that if there is a unitary operator $U'$ such that the probability of measuring a marked state upon measuring $U'^t|\Phi_0\rangle$ is $p > 0$, then there is a quantum procedure that finds the marked state with certainty using $O(1/\sqrt{p})$ applications of $U'^t$. That procedure uses the inversion about the mean, which can be implemented in $O(\sqrt{N})$ steps. This leads to an overall complexity of $O(\sqrt{N}\log N)$ for finding the marked state in the honeycomb lattice. This is the same complexity as the AKR spatial-search algorithm on the cartesian grid of a torus (Ambainis *et al.* 2005), where each site has four neighbouring sites and the $N$ sites form a lattice.

In a remarkable paper, Tulsi described a method for improving even further the probability of finding the marked vertex (Tulsi 2008). Consider a quantum circuit that implements operator $R_t$ followed by $U$ as defined in Equation (16). Tulsi introduced an extra qubit and defined a new one-step evolution operator as described in the circuit of Figure 2, where $-Z$ is the negative of the Pauli $Z$ operator and

$$X_\delta = \begin{pmatrix} \cos\delta & \sin\delta \\ -\sin\delta & \cos\delta \end{pmatrix}, \tag{30}$$

where $\delta$ must assume the value $1/\sqrt{\log N}$. It is straightforward to show that Tulsi's procedure increases the overlap between the final state and the target such that $|\langle t|\Phi_f\rangle| = O(1)$. Consequently, using Tulsi's modification, the overall time complexity of the search algorithm in the honeycomb lattice may be improved to $O(\sqrt{N\log N})$, as in the AKR case. It is not necessary to use the amplitude amplification method in this case. We have performed an independent numerical simulation that agrees with this analytical calculation.

https://doi.org/10.1017/S0960129510000332 Published online by Cambridge University Press

## 4. Conclusions

Hexagonal networks (honeycombs) are the underlying representation of a carbon structure called graphene, which has been attracting special attention in recent years, especially for its potential applications in nanotechnology. In this paper, we have discussed a new quantum algorithm for spatial search in a honeycomb with periodic boundary conditions. The protocol is based on a quantum walk in the honeycomb. We obtained the expression for the evolution operator in the Fourier representation and solved its eigenvalue problem. We then used the abstract search formalism developed in Ambainis *et al.* (2005) to obtain the complexity of the algorithm from the partially known spectral decomposition of the evolution operator. Our results have been verified by numerical simulations.

The search algorithm on the honeycomb has an overall time complexity of $O(\sqrt{N}\log N)$ using the amplitude amplification procedure. Further improvement, to $O(\sqrt{N\log N})$, can be obtained using Tulsi's technique. Surprisingly, this is the same complexity found for the quantum search on the square grid after Tulsi's improvement. Both the hexagonal grid and the square grid are regular graphs that cover the plane, although the former has degree 3 and the latter has degree 4. The fact that the complexity of the search algorithm is the same in both cases suggests that the number of connections of each node is not affecting the complexity of the abstract spatial search algorithm.

Several open questions remain. One of them is whether the abstract search algorithm has the same complexity when applied to graphs of general degrees. The triangular network, for instance, has degree 6 and also covers the plane. It would be interesting to investigate the behaviour of the algorithm on this topology. One may also inquire how robust the search algorithm is when there are some missing nodes. Finally, we point out that an optimal spatial search algorithm $O(\sqrt{N})$ for the case of a two-dimensional network covering the plane has not yet been found.

## Aknowledgements

We acknowledge helpful discussions with R. Marotti and R. Siri and thank M. Forets for help in revising the final version of the manuscript. This work was done with financial support from PEDECIBA (Uruguay) and CNPq (Brazil).

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