The Grover search as a naturally occurring phenomenon

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We provide the first evidence that under certain conditions, electrons may naturally behave like a Grover search, looking for defects in a material. 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. Some of these are well-known to recover the $(2+1)$–dimensional Dirac equation in continuum limit, i.e. the free propagation of the electron. We study two such Dirac QW, one on the square grid and the other on a triangular grid reminiscent of graphene-like materials. The numerical simulations show that the walker localises around a defect in $O(\sqrt{N})$ steps with probability $O(1/\log N)$. This in line with previous QW formulations of the Grover search on the 2D grid. But these Dirac QW are 'naturally occurring' and require no specific oracle step other than a hole defect in a material.

Quantum Computing has three main fields of applications for quantum computing : quantum cryptography ; quantum simulation ; and quantum algorithms (*e.g.* Grover, Shor...). Whilst the first two are considered short and mid term applications respectively, the last one, perhaps the most fascinating, is generally considered to be a long term application. This is because of the common understanding that we will need to build scalable implementations of universal quantum gate sets with fidelity 10^{-3} first, and implement quantum error corrections then, in order to finally be able to run our preferred quantum algorithm on the thereby obtained universal quantum computer. This seems feasible, yet long way to go.

In this letter we argue that this may be a pessimistic view. Scientists may get luckier than this and find out that nature actually implements some of these quantum algorithms 'spontaneously'. Indeed, the hereby presented research suggests that the Grover search may in fact be a naturally occurring phenomenon, when fermions propagate in crystalline materials under certain conditions.

Amongst all quantum algorithms, the reasons to focus on the Grover search [14] are many. First of all because of its remarkable generality, as it speeds up any brute force $O(N)$ problem into a $O(\sqrt{N})$ problem. Having just this quantum algorithm would already be extremely useful. Second of all, because of its remarkable robustness : the algorithm comes in many variants and has been rephrased in many ways, including in terms of resonance effects [23] and quantum walks [10].

Remember that a quantum walks (QW) are essentially local unitary gates that drive the evolution of a particle on a lattice. They have been used as a mathematical framework for different quantum algorithms [3, 27] but also for quantum simulations e.g. [4, 11, 13]. This is where things get interesting. Indeed, it has been shown many of these QW admit, as their continuum limit, some well-known PDE of physics, such as the Dirac equation [7, 12, 15, 21]. Recall that the Dirac equation governs the free propagation of the electron. Thus, these Dirac QW provided 'quantum numerical schemes', for the future quantum computers, to simulate the electron. For instance [17] shows that it is possible to describe the dynamics of fermions in graphene using QW. This is great, but now let us turn things the other way round : this also means that fermions provide a natural implementation of these Dirac QW. Could they be useful algorithmically ?

Here we provide evidence that these Dirac QW work fine to implement the diffusion step of the Grover search. Thus, fermions may provide a natural implementation of this step. However, recall that the Grover search is the alternation of a diffusion step, with an oracle step. The later puts on a minus one phase whenever the walker hits the solution of the problem. Could the oracle step be naturally implemented in terms of fermions, as well ? Here we provide evidence that the mere presence of hole defect suffices to implement an effective oracle step.

This paper focusses on Dirac QW in $(2+1)$–dimensions, on both the square grid and the triangular grid. The triangular grid is of particular interest for instance because of its ressemblance to several naturally occurring crystal-like materials. Moreover, it features topological phase effects which, by creating edge states around the hole defect, may help improbe localization. Notice the Grover search has already been described on triangular grids in [2, 9] and that, more generally, the Grover search has already been expressed as a QW on a variety of graphs before, yielding $O(\sqrt{N\log(N)})$ time complexity algorithms [1, 22, 25]. The aim of this contribution is to point out that simple variations of these are in fact naturally occurring phenomenon—with the hope to open a new and more direct route towards implementing the Grover search.

DIRAC QUANTUM WALKS

We consider QW both over the square and the triangular grid, i.e. a grid formed by tiling the plane regularly with equilateral triangles. Consider the line segments along which the facets of the squares (or triangles) are glued, and place a point in the middle. The walker lives on those points. For the square grid we may label these points by their positions in $\mathbb{Z}^2$, for the triangular grid this would be a subset of $\mathbb{Z}^2$. The walker's 'coin' or 'spin' degree of freedom lies in $\mathcal{H}_2$, for

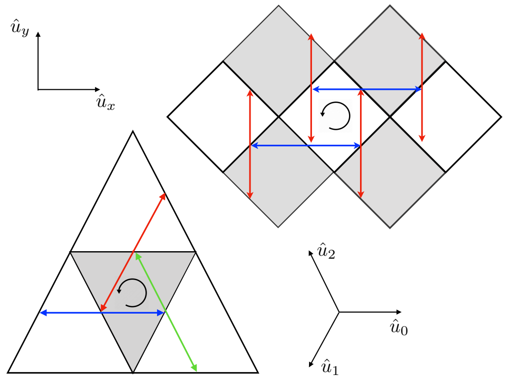

FIGURE 1: Quantum Walks scheme on triangular (left) and squared (right) lattice.

which we may chose some orthonormal basis $\{|v^-\rangle, |v^+\rangle\}$. The overall state of the walker lies in the composite Hilbert space $\mathcal{H}_2 \otimes \mathcal{H}_{\mathbb{Z}^2}$ and may be thus be written $|\psi\rangle = \sum_{\mathbf{x}} \psi^-(\mathbf{x}) |\mathbf{v}_-\rangle \otimes |\mathbf{x}\rangle + \psi^+(\mathbf{x}) |\mathbf{v}_+\rangle \otimes |\mathbf{x}\rangle$, where the scalar field ψ^- (resp. ψ^+) gives, at position $\mathbf{x} \in \mathbb{Z}^\mathbf{2}$, the amplitude of the particle being there and about to move backward (resp. forward) along a certain direction $\mathbf{u}$. We use $(t, \mathbf{x}) \in \mathbb{N} \times \mathbb{Z}^\mathbf{2}$, to label respectively instants and points in space and let the evolution operator be, in natural units :

$$|\psi(t+\varepsilon)\rangle = \Pi_i W_i T_{i,\varepsilon} |\psi(t)\rangle \tag{1}$$

with the set of coin-state-dependent discrete translation operators $T_{i,\varepsilon}$, each along directions $\mathbf{u_i}$, defined as :

$$T_{i,\varepsilon} \begin{pmatrix} \psi^+(\mathbf{x}) \\ \psi^-(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \psi^+(\mathbf{x} + \mathbf{u_i}\varepsilon) \\ \psi^-(\mathbf{x} - \mathbf{u_i}\varepsilon) \end{pmatrix}$$

and $W_i \in U(2)$. The QW we consider in this paper are Dirac QW, meaning that

$$\Pi_i W_i T_{i,\varepsilon} \approx \exp(i\varepsilon H_D) \tag{2}$$

as we neglect the second order terms in ε, and with H_D the Dirac Hamiltonian in some well-chosen representation and in $\hbar = c = 1$ units, e.g. $H_D = p_x\sigma_x + p_y\sigma_y + m\sigma_z$.

Square grid. Let us consider the unit vectors along the x–axis and y–axis, namely $\{\mathbf{u_x}, \mathbf{u_y}\}$ and use them to specify the directions of the translations $T_{x,\varepsilon}$ and $T_{y,\varepsilon}$. Eq. () then reads :

$$U = W_+ T_{y,\varepsilon} W_- T_{x,\varepsilon}$$

where $W_\pm = \exp(i\sigma_x\theta_\pm)$ with $\theta_\pm = \pm(\frac{\pi}{4} \pm \varepsilon m)$ and m a is real constant, namely the mass. In the formal limit for $\varepsilon \to 0$, the Eq. recovers the Dirac Hamiltonian in $(2+1)$–spacetime. Iterates of the walk converge towards solutions of the Dirac Eq., as was proven in full rigour in [6].

Triangular lattice. For the triangular lattice let us consider the unit vectors $\{\mathbf{u_0}, \mathbf{u_1}, \mathbf{u_2}\}$, as in Fig. 1 and defined by

$$\mathbf{u_k} = \cos\left(\frac{2k\pi}{3}\right)\mathbf{u_x} + \sin\left(\frac{2k\pi}{3}\right)\mathbf{u_y} \quad \text{for} \quad k = 0, 1, 2.$$

and use them to specify the directions of the translations $T_{i,\varepsilon}$. Eq. () then reads :

$$e^{-i\varepsilon H_D} = W T_{2,\varepsilon} W T_{1,\varepsilon} W T_{0,\varepsilon}$$

with $W = e^{i\frac{\pi}{3}} e^{-i\frac{\alpha}{2}\sigma_y} e^{-i\frac{\pi}{3}\sigma_z} e^{i\frac{\alpha}{2}\sigma_y} e^{-i\varepsilon\frac{3}{\sqrt{5}}m\sigma_z}$ the coin operator. In [5] it has been proved in detail by some of the authors how this particular choice also leads, in the continuum limit, to the Dirac Hamiltonian in $(2+1)$–spacetime.

Defects. A sector of a crystallographic lattice may be inaccessible, e.g. due to surface defects such as the vacancy of an atom (e.g. Schottky point defect) and others. These affect the physical and chemical properties of the material, including electrical resistivity or conductivity. In fact all real solids are impure with about one impurity per 10^6 atoms [16]. Here we model these defects in the simplest possible way : locally, a small number of squares or triangles are missing—thereby breaking the translation invariance of the lattice. In other words, the walker is forbidden access to a ball $\mathcal{B}$ of unit radius, as in Fig. 2. This is done by reflecting those signals that reach the boundary $\partial\mathcal{B}$ of the ball, simply by letting $W = \mathbb{I}_2$ on the facets around $\partial\mathcal{B}$.

Edge states. In both of these Dirac QW, one may notice that wherever we replace the coin W by identity, the walks reduce to just anti-clockwise rotation, see Fig. 1. Still, the operators and have different topological properties around $\partial\mathcal{B}$. The square lattice walk has vanishing Chern number and trivial topological properties [18], whereas the triangular walk has topologically non-trivial and Chern number equal to one [19]. In the triangular case the positive and negative component decouple respectively in the grey and the white triangles, and may be thought of as inducing polarized local topological currents of spin, called edge states [26]. According to [26], this phenomenon will be observed whenever initial states have an overlap with $\partial\mathcal{B}$, elsewhere the walker does not localize and explores the lattice with ballistic speed. Thus, we expect these topological effects to play a role in the triangular case only.

Our conjecture is that, starting from a uniformly superposed wavefunction, the walker will, in finite time, localise around the hole defect in $O(\sqrt{N})$ steps, with probability in $O(1/\log(N))$, with N the total number of squares/triangles. In the following we discuss the numerical evidence we have for such a conjecture.

GROVER SEARCH

Our numerical simulations over the square and triangular grids are exctly in line with a series of results [1, 10, 10, 25] showing that $2D$ spatial search can be performed in $O(\sqrt{N})$ steps with a probability of success in $O(1/\log N)$. With

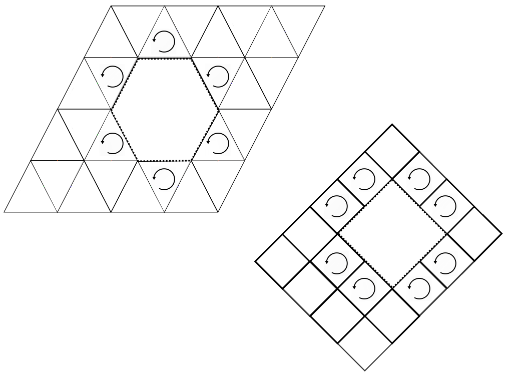

FIGURE 2: Hole defect in triangular (left) and squared (right) lattice.

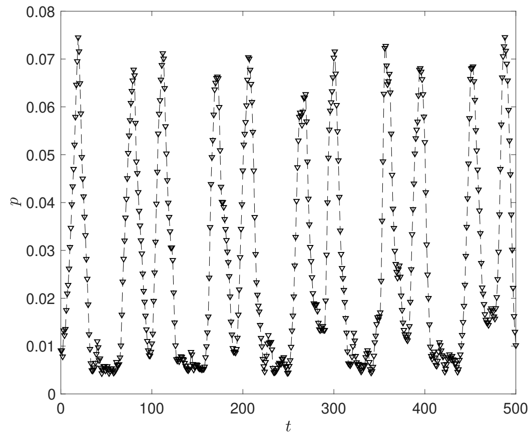

FIGURE 3: *Square grid periodic localization.* Probability of being localized around the center of the hole defect versus time. For $m = 0$ and $N = 2500$.

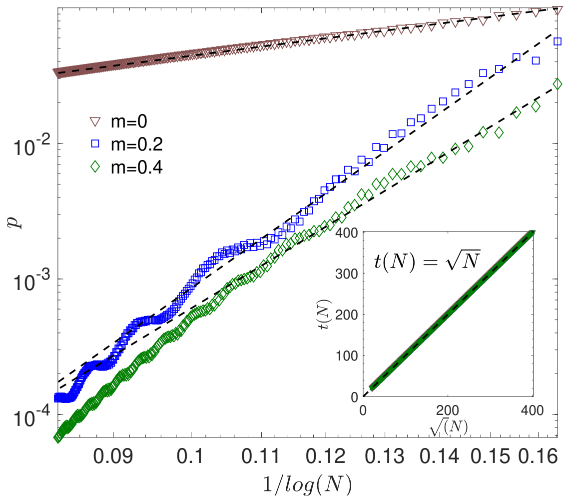

FIGURE 4: *Square grid scalings*. Peak probability of being localized around the hole defect, versus the number of squares in the grid. The inset shows the peak recurrence time.

$O(\log N)$ repetitions of the experiment one makes the success probability an $O(1)$, yielding an overall complexity of $O(\sqrt{N}\log N)$. Making use of quantum amplitude amplification [8], however, one just needs $O(\sqrt{\log N})$ repetitions of the experiment in order to make the probability an $O(1)$, yielding an overall complexity of $O(\sqrt{N\log N})$. This bound is unlikely to be improved, given the strong arguments given by [20]. In particular [22, 24] explain why the extra $\sqrt{\log N}$, with respect to Grover's original algorithm, is unlikely to be removed.

These work were not using Dirac QW, nor defects. Our aim here is demonstrate that QW which recover the Dirac equation, also perform a Grover search, as they propagate over the discrete surface and localise around its defects. More concretely we proceed as follows : (i) Prepare, as the initial state the wavefunction which is uniformly superposed ever every square or triangle, and whose coin degree of freedom is also the uniformly superposed $(|v^+\rangle + |v^-\rangle)/\sqrt{2}$. Notice that amplitude inside the hole defect is zero ; (ii) Let the walker evolve with time ; (iii) Quantify the number of steps t before the walker reaches its peak probability p of being localized in a ball of radius 2 around the center of the hole defect, and estimate this probability ; (iv) Characterize $t(N)$ and $p(N)$, i.e. the way the peak recurrence time and the peak probability depend upon the total number of squares/triangles N.
Indeed the probability of being found around the hole defect has a periodic behavior, see in Fig. 3 : for instance over a square lattice of $N = 2500$ sites, for $m = 0$, the peak recurrence time is $t = 50$, and the maximum probability is $p \simeq 10^{-1}$. The dependencies in N were interpolated from the data set shown Fig. 4, we observe that $t(N) = \sqrt{N}$ and $p(N) \simeq 1/\log N$, with a prefactor depending upon m. Clearly, repeating the experiment an $O(\log N)$ number of times will make the probability of finding the hole defect as close to 1 as desired, leading to an overall time complexity in $O(\sqrt{N}\log N)$. Again we could, instead, propose to use quantum amplitude amplification [8] in order to bring the needed number of repetitions down an $O(\sqrt{\log N})$, leading to an overall time complexity in $O(\sqrt{N\log N})$. But it seems that this would defeat the purpose of this paper to some extent : since our aim is to show that there is a 'natural implementation' of the Grover search, we must not rely on higher-level routines such as quantum amplitude amplification.

Over the triangular grid the situation is slightly more intricate, as two phenomena seem to coexist.
On the one hand, the Grover search is again at play. Indeed the data set of Fig. 5, confirms the results obtained over the square grid : the peak recurrence time is again $t(N) \simeq O(\sqrt{N})$, and its corresponding peak probability is again $p(N) \simeq O(1/\log N)$ for large N, although this time with a prefactor that depends upon the mass. Again this leads to an overall complexity of $O(\sqrt{N}\log N)$, or $O(\sqrt{N\log N})$ using amplitude amplification.

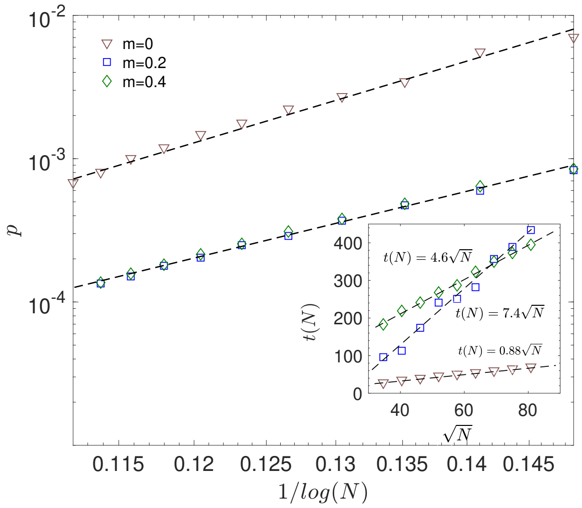

FIGURE 5: *Triangular grid scalings.* Recurring peak probability of being localized around the hole defect, versus the number of triangles in the grid. The inset shows the peak recurrence time.

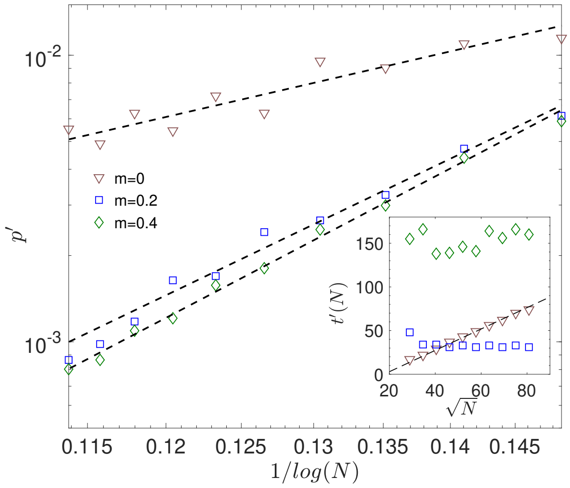

FIGURE 6: *Triangular grid edge states appearance.* First peak probability of being localized around the hole defect, versus the number of triangles in the grid. The inset shows the occurring time of this first peak.

On the other hand, a topological effect is at play. Indeed, an edge state rapidly appears, on the boundary $\partial\mathcal{B}$ of the hole defect. This first peak's probability also seems to scale as $p'(N) \simeq O(1/\log N)$, but with an occurrence time t'_m which is constant in N whenever $m > 0$. At first this seems extremely promising, suggesting that the hole defect may be found in $O(\log N)$, breaking Grover's optimality bound. On second thoughts one realizes that this is overoptimistic, and that this scaling cannot hold for large N. Indeed, if the first peak's occurrence time t'_m is constant, then its amplitude can only ever be drawn from the $\pi {t'_m}^2$ adjacent sites, each of which started with probability $1/N$. Summing them all yields $\pi {t'_m}^2/N$. Thus $p'(N)$ is, in the long run an $O(1/N)$: the first peak brings no complexity advantage. By augmenting the mass as a function of N, one can augment $t'_{m(N)}$ and escape this upper bound, but then $t'_{m(N)}$ needs again be an $O(\sqrt{N})$. Still, at the technical level it may be advantageous, for instance, to tune the mass so that $t'_{m(N)}$ equals $t(N)$ and have both the Grover search effect and the topological effect interfere constructively.

CONCLUSION

It is now common knowledge that Quantum Walks (QW) implement the Grover search, and that some QW mimic the free propagation of the electron. Yet, could this mean that free electrons naturally implement the Grover search ? Answering this question positively may be the path to a serious technological leap, whereby experimentalist would bypass the need for a full-fledged scalable and error-correcting Quantum Computer, and take the shortcut of looking for 'natural occurrences' of the Grover search instead.

So far, however, this idea has remained unexplored. The QW used to implement the Grover diffusion step had nothing to do with the Dirac QW used to simulate the electron. Moreover, the Grover oracle step seemed like a rather artificial, involved controlled-phase, far from something that could occur in nature. This contribution begins to remedy both these objections.

Indeed, we used Dirac QW over both the triangular and the square grid as the Grover diffusion step. Instead of alternating this with an extrinsic oracle step, we coded for the solution directly inside the grid, by introducing a hole defect. We obtained strong numerical evidence showing that the Dirac QW localize around the hole defect in $O(\sqrt{N})$ steps with probability $O(1/\log N)$, just like previous QW implementations of the Grover search would. We observed how sometimes topological effects come into play that may be of technical help.

Our next step is to use Dirac QW to locate not just a hole defect, but a particular QR code–like defect, amongst many possible others that could be present on the lattice. This would bring us one step closer to a natural implementation of an unstructured database Grover search.

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[1] Scott Aaronson and Andris Ambainis. Quantum search of spa-

tial regions. In *44th Annual IEEE Symposium on Foundations of Computer Science, 2003. Proceedings.*, pages 200–209. IEEE, 2003.

[2] G. Abal, R. Donangelo, M. Forets, and R. Portugal. Spatial quantum search in a triangular network. *Mathematical Structures in Computer Science*, 22(3) :521–531, June 2012. arXiv : 1009.1422.

[3] Andris Ambainis, Andrew M Childs, Ben W Reichardt, Robert Špalek, and Shengyu Zhang. Any and-or formula of size n can be evaluated in time n^1/2+o(1) on a quantum computer. *SIAM Journal on Computing*, 39(6) :2513–2530, 2010.

[4] Pablo Arrighi, Cédric Bény, and Terry Farrelly. A quantum cellular automaton for one-dimensional qed. *arXiv preprint arXiv :1903.07007*, 2019.

[5] Pablo Arrighi, Giuseppe Di Molfetta, Iván Márquez-Martín, and Armando Pérez. The Dirac equation as a quantum walk over the honeycomb and triangular lattices. *Physical Review A*, 97(6) :062111, June 2018. arXiv : 1803.01015.

[6] Pablo Arrighi, Vincent Nesme, and Marcelo Forets. The dirac equation as a quantum walk : higher dimensions, observational convergence. *Journal of Physics A : Mathematical and Theoretical*, 47(46) :465302, 2014.

[7] Iwo Bialynicki-Birula. Weyl, Dirac, and Maxwell equations on a lattice as unitary cellular automata. *Physical Review D*, 49(12) :6920–6927, June 1994.

[8] Gilles Brassard, Peter Hoyer, Michele Mosca, and Alain Tapp. Quantum amplitude amplification and estimation. *Contemporary Mathematics*, 305 :53–74, 2002.

[9] Bruno Chagas, Renato Portugal, Stefan Boettcher, and Etsuo Segawa. Staggered Quantum Walk on Hexagonal Lattices. *Physical Review A*, 98(5) :052310, November 2018. arXiv : 1806.10249.

[10] Andrew M Childs and Jeffrey Goldstone. Spatial search by quantum walk. *Physical Review A*, 70(2) :022314, 2004.

[11] Giuseppe Di Molfetta, Marc Brachet, and Fabrice Debbasch. Quantum walks in artificial electric and gravitational fields. *Physica A : Statistical Mechanics and its Applications*, 397 :157–168, 2014.

[12] Giuseppe Di Molfetta and Fabrice Debbasch. Discrete-time quantum walks : continuous limit and symmetries. *Journal of Mathematical Physics*, 53(12) :123302, 2012.

[13] Giuseppe Di Molfetta and Armando Pérez. Quantum walks as simulators of neutrino oscillations in a vacuum and matter. *New Journal of Physics*, 18(10) :103038, 2016.

[14] Lov K. Grover. A fast quantum mechanical algorithm for database search. In *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing - STOC '96*, pages 212–219, Philadelphia, Pennsylvania, United States, 1996. ACM Press.

[15] Mohamed Hatifi, Giuseppe Di Molfetta, Fabrice Debbasch, and Marc Brachet. Quantum walk hydrodynamics. *Scientific reports*, 9(1) :2989, 2019.

[16] Harald Ibach and Hans Lüth. *Solid-State Physics : An Introduction to Theory and Experiment*. Springer-Verlag, 1995.

[17] Ioannis G. Karafyllidis. Quantum walks on graphene nanoribbons using quantum gates as coins. *Journal of Computational Science*, Complete(11) :326–330, 2015.

[18] Takuya Kitagawa. Topological phenomena in quantum walks : elementary introduction to the physics of topological phases. *Quantum Information Processing*, 11(5) :1107–1148, 2012.

[19] Takuya Kitagawa, Mark S Rudner, Erez Berg, and Eugene Demler. Exploring topological phases with quantum walks. *Physical Review A*, 82(3) :033429, 2010.

[20] Frédéric Magniez, Ashwin Nayak, Peter C Richter, and Miklos Santha. On the hitting times of quantum versus random walks. *Algorithmica*, 63(1-2) :91–116, 2012.

[21] David A. Meyer. From quantum cellular automata to quantum lattice gases. *Journal of Statistical Physics*, 85(5-6) :551–574, December 1996. arXiv : quant-ph/9604003.

[22] Apoorva Patel, KS Raghunathan, and Md Aminoor Rahaman. Search on a hypercubic lattice using a quantum random walk. ii. d= 2. *Physical Review A*, 82(3) :032331, 2010.

[23] A. Romanelli, A. Auyuanet, and R. Donangelo. Quantum search with resonances. *Physica A : Statistical Mechanics and its Applications*, 360(2) :274 – 284, 2006.

[24] Miklos Santha. Quantum walk based search algorithms. In *International Conference on Theory and Applications of Models of Computation*, pages 31–46. Springer, 2008.

[25] Avatar Tulsi. Faster quantum-walk algorithm for the two-dimensional spatial search. *Physical Review A*, 78(1) :012310, 2008.

[26] Alberto D Verga. Edge states in a two-dimensional quantum walk with disorder. *The European Physical Journal B*, 90(3) :41, 2017.

[27] Guoming Wang. Efficient quantum algorithms for analyzing large sparse electrical networks. *Quantum Info. Comput.*, 17(11-12) :987–1026, September 2017.