Quantum walks on graphene nanoribbons using quantum gates as coins

Ioannis G. Karafyllidis *

Department of Electrical and Computer Engineering, Democritus University of Thrace, Kimmeria Campus, 67100, Xanthi, Greece

ARTICLE INFO

ABSTRACT

Both discrete and continuous quantum walks on graphs are universal for quantum computation. We define and use discrete quantum walks on the graphene honeycomb lattice to investigate the possibility of using graphene armchair and zigzag nanoribbons to implement quantum gates. The probability distribution of the quantum walker location represents the particle (electron) density distribution on the graphene lattice. We use a universal set of quantum gates as coins that drive the quantum walk and show that different quantum gates result in distinguishable particle distributions on the graphene lattice.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Quantum walks were initially introduced as quantizations of classical random walks [1,2]. Quantum walks represent quantum evolution in continuous spaces, discrete lattices and graphs by the motion of a quantum walker under the action of unitary operators, derived from the specific Hamiltonians [2,3]. Quantum walk theory has been developing rapidly and has become a powerful model for quantum system evolution with direct connections to Feynman propagators and quantum cellular automata [4–9]. Among others, quantum walks have been applied to solve decision problems in terms of quantum walks on decision trees, to model breakdown of electric field driven systems, to study nanotubules and to develop new quantum algorithms [10–13].

Quantum walks have been proven to be a universal model for quantum computation. Continuous quantum walks on graphs can encode any quantum computation with quantum gates implemented by scattering processes [14,15]. Discrete quantum walks have been proven to implement the same universal quantum gate set and thus are able to implement any quantum algorithm [16]. Quantum walks can also be encoded as quantum circuits, which is also a universal model for quantum computation [17,18].

Although both continuous and discrete quantum walks on graphs are universal models for quantum computation the authors of [14–16] do not suggest or explain how a physical quantum

computing system can be built based on the mathematical graph structures they propose. In the proposed quantum walk models, graphs and wires represent computational quantum basis states and not qubits and the models do not represent a physical quantum computer architecture. Mapping the quantum walk universal quantum computation model on a physical system is not an easy task, but if such a mapping can be achieved, the building of programmable quantum computing systems may be possible.

Graphene is a sheet of carbon atoms arranged in a honeycomb lattice. Because of its remarkable electronic properties, it has been proposed that graphene can serve as a physical platform for implementing quantum gates and circuits [19–20]. The possibility of implementing quantum dots, spin qubits, valley filters and valley valves has been studied with encouraging results [21–23].

In this paper, we investigate the possibility of using graphene nanostructures, such as nanoflakes and nanoribbons, to physically implement the universal quantum walk model. We define the discrete quantum walk on the two-dimensional hexagonal graphene lattice. In this discrete quantum walk, the quantum walker represents a particle (electron) moving in the lattice and the probability distribution of the walker location represents the electron density distribution on the graphene lattice. Instead of the usual Grover and quantum Fourier transform (QFT) coins, we use quantum gates as coins to drive the quantum walk. These coins (i.e. the quantum gates) represent physical actions of magnetic fields, electric fields and laser pulses on graphene nanostructures. We use a universal set of quantum gates, namely the Hadamard (H) gate, the phase-shift (P) gate and the controlled-not (CNOT) gate.

* Tel.: +30 2541079548.
E-mail address: ykar@ee.duth.gr
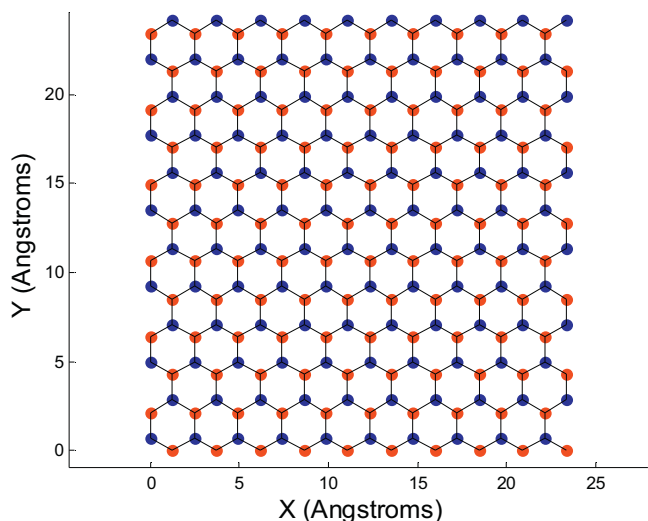
Fig. 1. A graphene nanoflake The honeycomb graphene lattice comprises two sublattices, indicated by red and blue. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Quantum walks on infinite lines and infinite regular graphs have been solved analytically [24,25], but it would be very difficult or even impossible to obtain analytical solutions for the various shapes of graphene nanostructures, mainly because of the non-infinite boundaries. Therefore, we develop an algorithm that simulates the quantum walk on finite hexagonal graphene lattices and compare the various particle distributions on different graphene nanostructure lattices. We conclude that these distributions are distinguishable and that it is worthy to further study graphene as a physical quantum computing platform, using both theoretical and experimental methods.

2. Definition of the quantum walk on the graphene lattice

Graphene lattice is not a Bravais lattice and its unit cell comprises two carbon atoms. The repetition of these atoms form two sulattices which are shown in Fig. 1. In the graphene nanoflake shown in this figure, the atoms belonging to different sulattices are indicated with different colors, red and blue. The distance between two neighboring atoms is 1.42 Å. Two carbon atoms belonging to
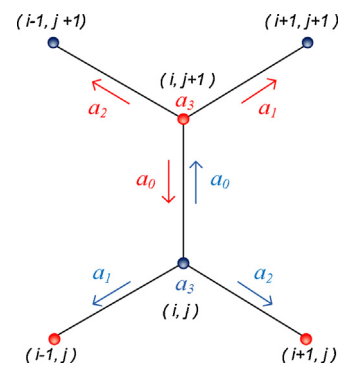
Fig. 3. Motion of the quantum walker and the corresponding quantum coin amplitudes a_0, a_1, a_2 and a_3. The indices i and j give the position of the atom in the lattice. (For interpretation of the references to colour in the text, the reader is referred to the web version of this article.)

different sublattices are not equivalent, because the lattice looks different from these atom sites.

Fig. 2 shows two graphene nanoribbons. The shape of the nanoribbon border determines the carrier velocity in graphene. Fig. 2a shows a zigzag and Fig. 2b shows an armchair nanoribbon.

Fig. 3 shows two atoms belonging to the two sublattices, the blue *(i,j)* and the red *(i,j + 1)*, and their neighbors. Note that atoms in the same zigzag line along the *x*-axis are indicated with the same *j* index. We associate a quantum coin to each atom in the graphene lattice. The quantum coin state $|c\rangle$ spans a Hilbert space, the coin space Hc, and has four probability amplitudes:

$$|c\rangle = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} \qquad (1)$$

These four amplitudes are associated with the direction of motion of the quantum walker (particle) from the current atom to each one of its neighbors, as shown in Fig. 3. Amplitude a_3 is the amplitude associated with the particle staying at the atom where it is currently located. The atom positions define another basis for the quantum walk in which the state $|i, j\rangle$ represents the quantum walker positioned at the atom (i, j). These states span the position Hilbert space
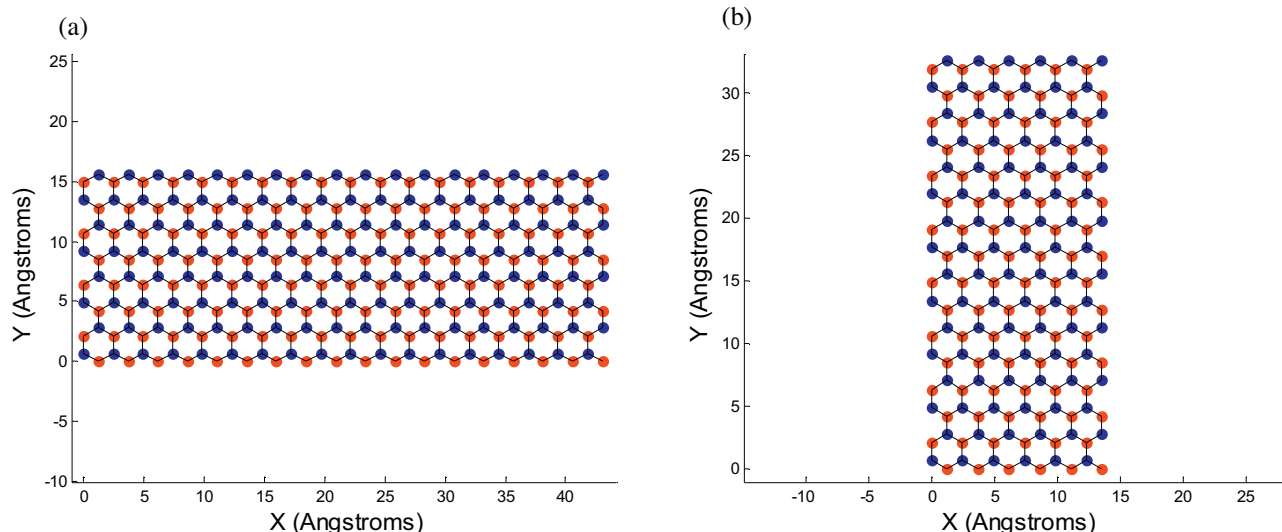
Fig. 2. (a) A zigzag graphene nanoribbon. (b) An armchair graphene nanoribbon.