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Construction of distinct discrete time scattering quantum walk formulations on the honeycomb lattice

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ABSTRACT

Here we address the scattering construction of discrete time quantum walks on the honeycomb lattice. We write the system general (unitary) one step time evolution operator in terms of: (i) complete arbitrary scattering matrices $\Gamma^{(j,k)}$, defined on the sites (j, k) of the lattice and; and (ii) topological directional functions Φ, which represent the distinct ways we can keep track of the propagation directions along the three bonds attached to each (j, k). By imposing the Φ's to comply with all the honeycomb translational and point group symmetries (in the case of $\Gamma^{(j,k)} = \Gamma$), we obtain in total ten independent model versions, presenting different dynamical features. To study some of their traits, we consider the idea of 'characteristic paths' CPs (closely related to classical random walks), determining the CPs for each one of the ten formulations. We then discuss many numerical examples of time evolution dynamics for our scattering quantum walks. For the calculations we use few Γ's, as the Discrete Fourier Transform (DFT) and Grover matrices.

1. Introduction

Random walks (RWs) in general [1] and Brownian motion in particular [2] are long-established important subjects in the realm of classical physics, encompassing a broad range of applications [3]. In the most basic 1D formulation, a RW is a simple stochastic dynamics where a particle (leaving from $x = x_0$ at $t = 0$) continuously moves with constant speed, $v > 0$, in the infinite line. Defining $\ell = v\,\tau$ – for τ a characteristic time – each time (at $t = \tau, t = 2\tau, t = 3\tau, \ldots$) the particle reaches a

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position $x_j = x_0 + j\,\ell$ ($j \in \mathbb{Z}$), an instantaneous decision about the next direction to go (either right, with probability p, or left, with $1 - p$) is made. Thus, once in x_j the particle immediately switches or not the velocity signal according to such choice. In this way, the classical RW can be viewed as taking place in a 'lattice' (or graph), with the 'sites' (or vertices) located at the x_j's and separated by 'bonds' (or edges) of length ℓ. Hence, we have a random process at the vertices and a deterministic movement along the edges [4].

The explicit idea[1] of quantum walks[2] (QWs) first appeared in 1993 [7] as a possible quantum version of classical RWs (see also [8]). Nowadays the concept has been largely extended [9–11], although still being based on the above classical RW picture of an underlying lattice structure. QWs are commonly defined on discrete spaces (graphs) and classified into two groups, depending on whether time is a continuous [12] or a discrete variable [13]. For the discrete case – our focus here – the two main formulations (although unitarily equivalent [4,14,15]) are the coin and scattering models. Very briefly, coin QWs (CQWs) consist of unitary quantum evolutions for systems whose Hilbert space eigenbasis can be associated to the vertices of a graph. Furthermore, 'inner' degrees of freedom (similar to spins) play the role of coin states $|\sigma\rangle$, responsible for directing (through the action of proper coin operators on these $|\sigma\rangle$) the propagation of a state $|\psi_{n-1}\rangle$ (for $n = 1, 2, \ldots$) along the graph vertices, resulting in $|\psi_n\rangle$ [13].

The version we shall address in this contribution are scattering QWs (SQWs). In this case, the dynamics is defined on the graph edges (lattice bonds) and at any time step the state suffers scattering due to the graph vertices (lattice sites). In fact, at time step n the system full $|\psi_n\rangle$ is written as the superposition of the basis states – associated to the individual bonds – 'weighted' by the transmission and reflection amplitudes — associated to the distinct sites scattering matrices [14]. This formal construction has a nice analogy with light beams in an interferometric network. Each site acts as a beam splitter and the edges are like optical axis (allowing propagation in both directions). Also, each beam splitter can be attached to a different number of optical axis, so the web does not need to be regular. A brief review of SQWs mathematical description (in the 1D case) is presented in Section 2.

Given their relative simplicity – compared to more 'traditional' quantum system models – but yet displaying most of the basic phenomenology associated to quantum mechanics [16–20], QWs find innumerous usages [9,11,21]. For instance, it has been shown that primitive quantum computers could be fully based on QWs [22–24]. So, they are relevant tools in the development of algorithms for quantum computation [10]. Other examples of problems addressed as QWs are: electronic transport in different materials [25,26], photosynthetic processes [27,28], disorder in non-interacting bosonic and fermionic systems [29], quantum phase transition in optical traps [30], spin states transfer in interacting systems [31], Bose–Einstein condensates [32], and percolation graphs [33,34], to name just a few. As for actual physical implementation, concrete QWs have been proposed in terms of photon interferometers [35] and waveguides [36–38], neutral atoms [39–41] and ions [42–44] trapped in optical lattices, quantum dots [45], and nuclear-magnetic-resonance processors [46].

Most of the foreseen applications and experimental constructions for QWs are thought for the 1D case, in which from any site there are only two possible "directions to go" (so, the coordination number is $k = 2$). Nonetheless, effects like topological phases and transitions observed in 1D [47–50] conceivably would display a broader range of features in structures with $k > 2$, specially for k odd [51] (as explicit examples for $k = 3$ see, e.g., [52–54]). Moreover, different works have demonstrated a much richer phenomenology for QWs in two and higher dimensions, as in square ($k = 4$) and hypercube ($k = 2N$ for ND) lattices [4,55–59]. In fact, as pointed out in [60], QWs are natural models to describe electronic excitations (of proper wave numbers[3]) in distinct crystalline lattices [61].

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[1] Interestingly, the quantum walk concept is somehow already present in Feynman's pioneer work discretizing the kernel of the Dirac equation, see, e.g., [5]. Also, a similar construction to quantum walks has been proposed in 1996 [6], but in the context of the quantum cellular automata.

[2] The original term proposed in [7] was "quantum random walks", but today the more usual practice is to call such family of systems just "quantum walks".

[3] Basically, the wavelengths must be small enough so that the 'local' topology (i.e., that around individual sites) becomes relevant for the transport properties.