# SCIENTIFIC REPORTS

Received: 12 October 2017 Accepted: 16 May 2018 Published online: 22 June 2018

## **QUANTUM walks on regular uniform hypergraphs**

**Ying Liu , Jiabin Yuan, Bojia Dua[n](http://orcid.org/0000-0003-1263-8047) & Dan Li**

**Quantum walks on graphs have shown prioritized benefts and applications in wide areas. In some scenarios, however, it may be more natural and accurate to mandate high-order relationships for hypergraphs, due to the density of information stored inherently. Therefore, we can explore the potential of quantum walks on hypergraphs. In this paper, by presenting the one-to-one correspondence between regular uniform hypergraphs and bipartite graphs, we construct a model for quantum walks on bipartite graphs of regular uniform hypergraphs with Szegedy's quantum walks, which gives rise to a quadratic speed-up. Furthermore, we deliver spectral properties of the transition matrix, given that the cardinalities of the two disjoint sets are diferent in the bipartite graph. Our model provides the foundation for building quantum algorithms on the strength of quantum walks on hypergraphs, such as quantum walks search, quantized Google's PageRank, and quantum machine learning.**

As a quantum-mechanical analogs of classical random walks, quantum walks have become increasingly popular in recent years, and have played a fundamental and important role in quantum computing. Owing to quantum superpositions and interference efects, quantum walks have been efectively used to simulate quantum phe-nomena<sup>1</sup>, and realize universal quantum computation<sup>[2](#page-6-1),[3](#page-6-2)</sup>, as well as develop extensively quantum algorithms<sup>[4](#page-6-3)</sup>. A wide variety of discrete quantum walk models have been successively proposed. The first quantization model of a classical random walk, which is the coined discrete-time model and which is performed on a line, was proposed by Aharonov $^5$  $^5$  in the early 1990s. Aharonov later studied its generalization for regular graphs in ref. $^6$  $^6$ . Szegedy $^7$  $^7$ proposed a quantum walks model that quantizes the random walks, and its evolution operator is driven by two refection operators on a bipartite graph. Moreover, in discrete models, the most-studied topology on which quantum walks are performed and their properties studied are a restricted family of graphs, including line<sup>8,[9](#page-7-1)</sup>, cycle<sup>10,11</sup>, hypercube<sup>12,13</sup>, and general graphs<sup>[14](#page-7-6)[–17](#page-7-7)</sup>. Indeed, most of the existing quantum walk algorithms are superior to their classical counterparts at executing certain computational tasks, e.g., element distinctness<sup>18,19</sup>, trian-gle finding<sup>20,21</sup>, verifying matrix products<sup>22</sup>, searching for a marked element<sup>16,23</sup>, quantized Google's PageRank<sup>[24](#page-7-15)</sup> and graph isomorphism<sup>[25](#page-7-16),[26](#page-7-17)</sup>. In addition to above scientific documents, there are many good introductions and reviews written by Kempe<sup>27</sup>, Kendon<sup>28,29</sup>, Venegas-Andraca<sup>30</sup>, and Wang<sup>31</sup> relevant to deepening into the physical, mathematical and algorithmic properties of quantum walks.

In mass scenarios, a graph-based representation is incomplete, since graph edges can only represent pairwise relations between nodes. However, hypergraphs are a natural extension of graphs that allow modeling of higher-order relations in data. Because the mode of representation is even nearer to the human visual grouping system, hypergraphs are more available and efective than graphs for solving many problems in several applications. Owing to Zhou's random walks on hypergraphs for studying spectral clustering and semi-supervised rank-ing<sup>32</sup>, hypergraphs have made recent headlines in computer vision<sup>[33](#page-7-24),[34](#page-7-25)</sup>, information retrieval<sup>35–37</sup>, and categorical data clustering<sup>[38](#page-7-28)</sup>. Many interesting and promising findings were covered in random walks on hypergraphs, and quantum walks provide a method to explore all possible paths in a parallel way, due to constructive quantum interference along the paths. Terefore, paying attention to quantum walks on hypergraphs is a natural choice.

Inspired by these latter developments, we focus on discrete-time quantum walks on regular uniform hyper-graphs. In ref.<sup>[39](#page-7-29)</sup>, Konno defined a two-partition quantum walk and the quantum walk on hypergraph, also he showed that the quantum walk on hypergraph is also a two partition quantum walk. In this paper, by analyzing the mathematical formalism of hypergraphs and three existing discrete-time quantum walks<sup>40</sup> (coined quantum walks, Szegedy's quantum walks, and staggered quantum walks), we fnd that discrete-time quantum walks on regular uniform hypergraphs can be transformed into Szegedy's quantum walks on bipartite graphs that are used

Nanjing University of Aeronautics and Astronautics, College of Computer Science and Technology, Nanjing, 211106, China. Correspondence and requests for materials should be addressed to Y.L. (email: [lycherish@nuaa.edu.cn](mailto:lycherish@nuaa.edu.cn)) or J.Y. (email: [jbyuan@nuaa.edu.cn](mailto:jbyuan@nuaa.edu.cn))

to model the original hypergraphs. Furthermore, the mapping is one to one. That is, we can study Szegedy's quantum walks on bipartite graphs instead of the corresponding quantum walks on regular uniform hypergraphs. In ref[.7](#page-6-6) Szegedy proved that his schema brings about a quadratic speed-up. Hence, we construct a model for quantum walks on bipartite graphs of regular uniform hypergraphs with Szegedy's quantum walks. In the model, the evolution operator of an extended Szegedy's walks depends directly on the transition probability matrix of the Markov chain associated with the hypergraphs.

In more detail, we frst introduce the classical random walks on hypergraphs, in order to get the vertex-edge transition matrix and the edge-vertex transition matrix. We then defne a bipartite graph that is used to model the original hypergraph. Lastly, we construct quantum operators on the bipartite graph using extended Szegedy's quantum walks, which is the quantum analogue of a classical Markov chain. In this work, we deal with the case that the cardinalities of the two disjoint sets can be diferent from each other in the bipartite graph. In addition, we deliver a slightly diferent version of the spectral properties of the transition matrix, which is the essence of the quantum walks. As a result, our work generalizes quantum walks on regular uniform hypergraphs by extending the classical Markov chain, due to Szegedy's quantum walks.

The paper is organized as follows. There three subsection in Sec. Results. In Sec. Results: *Random walks on hypergraphs*, we briefy introduce random walks on hypergraphs needed to present the quantum version of it. In Sec. Results: *Quantum walks on hypergraphs*, we construct a method for quantizing Markov chain to create discrete-time quantum walks on regular uniform hypergraphs. In Sec. Results: *Spectral analysis of quantum walks on hypergraphs*, we analyze the eigen-decomposition of the operator. Sec. Discussion is devoted to conclusions.

#### **Results**

**Random walks on hypergraphs.** Let *HG*=(*V*, *E*) denote a hypergraph, where *V* is the vertex set of the hypergraph and  $E \subset 2^V \setminus \{\{\}\}\$ is the set of hyperedges. Let  $V = \{v_1, v_2, ..., v_n\}$  and  $E = \{e_1, e_2, ..., e_m\}$ . where  $n = |V|$ is used to denote the number of vertices in the hypergraph and  $m=|E|$  the number of hyperedges. Given a hypergraph, define its incidence matrix  $H \in R^{n \times m}$  as follows:

$$
h(i, j) = \begin{cases} 1 & \text{if } v_i \in e_j \\ 0 & \text{if } v_i \notin e_j \end{cases}.
$$
 (1)

Then, the vertex and hyperedge degrees are defined as follows:

$$
d(\nu) = \sum_{e \in E} h(\nu, e) = |E(\nu)|,
$$
\n(2)

$$
E(\nu) = \{e \in E: \nu \in e\},\tag{3}
$$

$$
\delta(e) = \sum_{v \in V} h(v, e) = |e|,\tag{4}
$$

where  $E(v)$  is the set of hyperedges incident to *v*. A hypergraph is  $d$  – *regular* if all its vertices have the same degree. Also, a hypergraph is *k* – *uniform* if all its hyperedges have the same cardinality. In this paper, we will restrict our reach to quantum walks on *d* – *regular* and *k* – *uniform* hypergraphs from now on, denoting them as *HGk*,*<sup>d</sup>*.

A random walk on a hypergraph *HG*=(*V*, *E*) is a Markov chain on the state space *V* with its transition matrix *P*. The particle can move from vertex  $v_i$  to vertex  $v_j$  if there is a hyperedge containing both vertices. According to ref.[32,](#page-7-23) a random walk on a hypergraph is seen as a two-step process. First, the particle chooses a hyperedge *e* incident with the current vertex  $v$ . Then, the particle picks a destination vertex  $u$  within the chosen hyperedge satisfying the following:  $v, u \in e$ . Therefore, the probability of moving from vertex  $v_i$  to  $v_j$  is:

$$
P_{ij} = P(\nu_i, \nu_j) = \sum_{k=1}^{m} \frac{h_{ik} h_{jk}}{d(\nu_i) \delta(e_k)} = \frac{1}{d(\nu_i)} \sum_{k=1}^{m} \frac{h_{ik} h_{jk}}{\delta(e_k)},
$$
\n(5)

or, more accurately, the equation can be written as

$$
P = \sum_{\substack{e \in E, \\ \{v, u\} \subseteq e}} \frac{1}{d(v)\delta(e)} = \frac{1}{d(v)} \sum_{\substack{e \in E, \\ \{v, u\} \subseteq e}} \frac{1}{\delta(e)}.
$$
\n(6)

Let  $P_{VE}$  denote the vertex-edge transition matrix

$$
P_{VE} = D_{\nu}^{-1}H\tag{7}
$$

and  $P_{EV}$  the edge-vertex transition matrix

$$
P_{EV} = D_e^{-1} H^T \tag{8}
$$

with transition probability

$$
\sum_{e \in E} p_{ve} = 1, \forall v \in V,
$$
\n(9)



<span id="page-2-0"></span>**Figure 1.** Example of a hypergraph with six vertexes and four hyperedges, and its associated bipartite graph.

$$
\sum_{v \in V} p_{ev} = 1, \forall e \in E,
$$
\n(10)

where  $D<sub>v</sub>$  and  $D<sub>e</sub>$  are the diagonal matrices of the degrees of the vertices and edges, respectively. Naturally, we can indicate *P* in matrix form, as

$$
P = D_v^{-1} H D_e^{-1} H^T = P_{VE} P_{EV},
$$
\n(11)

**Quantum walks on hypergraphs.** In this section, we design quantum walks on regular uniform hypergraphs by means of Szegedy's quantum walks. We frst convert the hypergraph into its associated bipartite graph, which can be used to model the hypergraph. We then defne quantum operators on the bipartite graph using Szegedy's quantum walks, which are a quantization of random walks.

*Derving Bipartite graphs from hypergraphs*. Proposition 1Any regular uniform hypergraph *HGk*,*<sup>d</sup>* can be represented usefully by a bipartite graph  $BG_{n,m}$ : the vertices *V* and the edges *E* of the hypergraph are the partitions of BG, and  $(v_i, e_j)$  are connected with an edge if and only if vertex  $v_i$  is contained in edge  $e_j$  in HG.

*Proof.* Hypergraph can be described by binary edge-node incidence matrix *H* with elements (1). To the incidence matrix of a regular uniform hypergraph  $HG_{k,d}$  corresponds a bipartite incidence graph  $B(H) = G(V \cup E, E_B)$ which is defined as follows. The vertices *V* and the edges *E* of the hypergraph are the partitions of *BG*, and  $(v_i, e_j) \in E_B$  iff  $h_{ij} = 1$ . It is evident that B is bipartite, and the biadjacency matrix describing  $B(H)$  is the following  $(n+m) \times (n+m)$  matrix:

$$
A_B = \begin{pmatrix} 0 & H \\ H^T & 0 \end{pmatrix}.
$$
 (12)

Under this correspondence, the biadjacency matrices of bipartite graphs are exactly the incidence matrices of the corresponding hypergraphs.

A similar reinterpretation of adjacency matrices may be used to show a one-to-one correspondence between regular uniform hypergraphs and bipartite graphs. That is, discrete-time quantum walks on regular uniform hypergraphs can be transformed into quantum walks on bipartite graphs that are used to model the original hypergraphs. The transformation process is outlined in detail below. If there is a hyperedge  $e_k$  containing both vertices  $v_i$  and  $v_j$  in the original hypergraph  $HG = (V, E)$ , convert it into two edges  $(v_i, e_k)$  and  $(e_k, v_j)$  in the bipartite graph.

As a concrete example, we consider a 3 – *uniform* and 2 – *regular* hypergraph with the vertexes set  $V = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8, v_9, v_{10}\}$  $v_3$ ,  $v_4$ ,  $v_5$ ,  $v_6$ } and the set of hyperedges  $E = \{e_1, e_2, e_3, e_4\}$ . Then, a bipartite graph  $BG_{6.4}$  with partite sets  $V = \{v_1, v_2, v_3, v_4, v_5, v_6\}$  $v_3$ ,  $v_4$ ,  $v_5$ ,  $v_6$ } and  $E = \{e_1, e_2, e_3, e_4\}$  can represent the hypergraph  $H\hat{G}_{3,2}$ , which is depicted in Fig. [1](#page-2-0). Theorem 1Let  $HG = (V, E)$  be a hypergraph, and we have

$$
\sum_{v \in V} d(v) = \sum_{e \in E} d(e).
$$
\n(13)

*Proof.* Let  $B(H) = G(V \cup E, E_B)$  be the incidence graph of  $HG = (V, E)$ . We sum the degrees in the part *E* and in the part *V* in *B*(*H*). Since the sums of the degrees in these two parts are equal, we obtain the result. In particular, if the hypergraph is *d* – *regular* and *k* – *uniform*, we obtain *nd*=*mk*.

*Szegedy quantum walks on the bipartite graphs.* Since we have transformed the hypergraph *HGk*,*<sup>d</sup>* into its bipartite graph  $BG_{n,m}$ , we now describe Szegedy quantum walks that take place on the obtained bipartite graph  $BG_{n,m}$ by extending the class of possible Markov chains. The quantum walks on the hypergraph *HG* start by considering an associated Hilbert space that is a linear subspace of the vector  $H^{n^2m}=H^n_v\otimes H^m_e\otimes H^n_v,$  where  $n=|V|,$ an associated Theori space that is a mean subspace of the vector  $H = H_v \otimes H_e \otimes H_v$ , where  $h = |v|$ ,<br>  $m = |E|$ . The computational basis of  $H^{n^2m}$  is  $\{|v_i, e, v_j\rangle : e \in E$ ,  $v_i, v_j \in V$ ,  $v_j, v_j \in e\}$ . In addition, quantum walks on the bipartite graph  $BG_{n,m}$  with biadjacent matrix (12) have an associated Hilbert space  $H_A = H_v^n \otimes H_e^m$  and  $H_B = H_e^m \otimes H_v^n$ .

To identify quantum analogues of Markov chains - that is, the classical random walks with probability matrices (7) and (8) with entries of (9) and (10) - we define the vertex-edge transition operators:  $A: H^n \to H^{nd}$  and edge-vertex transition operators: *B*:  $H^m \to H^{mk}$  as follows:

$$
A = \sum_{v \in V} |\alpha_v\rangle\langle v|,\tag{14}
$$

$$
B = \sum_{e \in E} |\beta_e\rangle\langle e|,\tag{15}
$$

where

$$
\alpha_{\nu}\rangle = |\nu\rangle \otimes \left(\sum_{e \in E} \sqrt{P_{\nu e}} |e\rangle\right),\tag{16}
$$

$$
|\beta_e\rangle = \left(\sum_{v \in V} \sqrt{p_{ev}} |e\rangle\right) \otimes |\nu\rangle. \tag{17}
$$

The transition operators are defined on the Hilbert space  $H_A$  and  $H_B$  separately, where the computational basis of  $H^{nd}$  is  $\{ |v, e\rangle : v \in V, e \in E \}$  and the computational basis of  $H^{mk}$  is  $\{ |e, v\rangle : e \in E, v \in V \}$ . The states  $|\alpha_v\rangle$  and  $|\beta_e\rangle$ as superpositions that start from vertex *v* to hyperedge *e* and from hyperedge *e* to vertex *v*, respectively. Obviously, the dimensions of *A* and *B* are  $nd \times n$  and  $mk \times m$ , respectively. Note that  $nd = mk$  from theorem 1. Using (16) and (17) along with (9) and (10), we obtain the following properties:

$$
\langle \alpha_{\nu} | \alpha_{\nu'} \rangle = \delta_{\nu \nu'}, \tag{18}
$$

$$
\langle \beta_e | \beta_{e'} \rangle = \delta_{ee'}, \tag{19}
$$

as well as

$$
A^T A = I_n, \tag{20}
$$

$$
B^T B = I_m. \tag{21}
$$

One can easily verify that  $|\alpha_v\rangle$  and  $|\beta_e\rangle$  are unit vectors due to the stochasticity of  $P_{VE}$  and  $P_{EV}$ . Distinctly, these equations imply that the action of *A* preserves the norm of the vectors. The same is true regarding *B*.

<span id="page-3-0"></span>We now immediately define the projectors  $\Pi_A$  and  $\Pi_B$  as follows:

$$
\Pi_A = AA^T = \sum_{v \in V} |\alpha_v\rangle \langle \alpha_v|,\tag{22}
$$

$$
\Pi_B = BB^T = \sum_{e \in E} |\beta_e\rangle\langle\beta_e|.
$$
\n(23)

<span id="page-3-1"></span>Using Eqs ([22](#page-3-0)) and ([23](#page-3-1)), it is easy to see that  $\Pi_A$  projects onto subspace  $H_A$  spanned by  $\{|\alpha_v\rangle : v \in V\}$ , and  $\Pi_B$ projects onto subspace  $H_B$  spanned by  $\{|\beta_e\rangle: e \in E\}$ . After obtaining the projectors, we can define the associated refection operators, which are

$$
R_A = 2\Pi_A - I_{nd},\tag{24}
$$

$$
R_B = 2\Pi_B - I_{mk},\tag{25}
$$

where  $I_{nd} = I_{mk}$  is the identity operator.

Note that the reflection operators  $R_A$  and  $R_B$  are unitary, we can get the following Proposition.

Proposition 2 $R_A$  is a reflection operator about the space  $H_A$ . Similarly,  $R_B$  is a reflection operator about the space  $H_B$ . *Proof.* We prove that  $R_A$  is a reflection operator about the space  $H_A$ . The other claim is analogous.

$$
R_A|\Psi\rangle = (2\Pi_A - I)|\Psi\rangle
$$
  
= 
$$
\begin{cases} 2\sum_{v \in V} |\alpha_v\rangle \langle \alpha_v| - I | \Psi \rangle \\ = \begin{cases} |\Psi\rangle & \text{if } \Psi \in H_A \\ -|\Psi\rangle & \text{if } \Psi \in H_A^{\perp} \end{cases} \end{cases}
$$
 (26)

Defnition 1(**Quantization of M**.**C**. *P*)

$$
W = R_B R_A \tag{27}
$$

A single step of the quantum walks is given by the unitary evolution operator *W* based on the transition matrix *P*. In the bipartite graph, an application of *W* corresponds to two quantum steps of the walk from *v* to *e* and from *e* to *v*. At time *t*, the whole operator of the quantum walks is *Wt* .

**Spectral analysis of quantum walks on hypergraphs.** In many classical algorithms, the eigen-spectrum of the transition matrix *P* plays a critical role in the analysis of Markov chains. In a similar way, we now proceed to study the quantitative spectrum of the quantum walks unitary operator *W*.

Szegedy proved a spectral theorem for quantum walks,  $W = ref_2ref_1$ , in ref.<sup>[7](#page-6-6)</sup>. In this section, we deliver a slightly diferent version in that the cardinality of set *X* may be diferent from the cardinality of set *Y* in the bipartite graph. In order to analyze the spectrum, we need to study the spectral properties of an  $n \times m$  matrix *D*, which indeed establishes a relation between the classical Markov chains and the quantum walks. This matrix is defined as follows:

**Definition 2** (Discriminant Matrix) The discriminant matrix for *W* is

$$
D_{nm} = A^T B \tag{28}
$$

It also follows from the definition that  $D = \sqrt{P_{VP} \circ P_{EV}}$  with entries

$$
D_{ve} = \sqrt{p_{ve}p_{ev}}, \forall \ v \in V, \forall \ e \in E. \tag{29}
$$

Suppose that the discriminant matrix *D* has the singular value decomposition  $D = U \Sigma V^T = \sum_i \sigma_i \mu_i \nu_i^T$ . The left singular vectors  $|\mu_k\rangle$  satisfy

$$
D|\nu_k\rangle = \sigma_k|\mu_k\rangle \tag{30}
$$

and the right singular vectors

$$
\mu_k|D = \langle \nu_k|\sigma_k \tag{31}
$$

with  $\sigma_k$  the singular value.

**Theorem 2** For any  $\sigma_k$  the singular value of *D*,  $0 \le \sigma_k \le 1$ .

*Proof.* First, let  $Dk = \sigma_k k$ . Then we obtain

$$
\sigma_k|^2 ||k||^2 = ||Dk||^2
$$
  
=  $\langle Dk, Dk \rangle$   
=  $\langle A^T Bk, A^T Bk \rangle$   
=  $\langle Bk, AA^T Bk \rangle$   
 $\leq \langle Bk, Bk \rangle$   
=  $\langle k, B^T Bk \rangle$   
=  $\langle k, k \rangle = ||k||^2$ . (32)

Thus,  $|\sigma_k| \leq 1$ . Since  $\langle k, D^T D k \rangle \geq 0$  for all *k*, we have  $0 \leq \sigma_k$ . Therefore,  $0 \leq \sigma_k \leq 1$ .

Observing theorem 2, we can write the singular value  $\sigma_k$  as  $\cos \theta_k$ , where  $\theta_k$  is the principal angle between subspace  $H_A$  and  $H_B$ . In the earlier years, Björck and Golub<sup>[41](#page-7-31)</sup> deducted the relationship between the singular value decomposition and the principal angle  $\theta_k$  between subspace  $H_A$  and  $H_B$ . That is,  $cos(\theta_k) = \sigma_k$ .

In the remainder of this section, we will explore the eigen-decomposition of the operator *W*, which can be calculated from the singular value decomposition of *D*.

First, we turn to the dimensionality of the spaces. Suppose that *n*≥*m*. We learned earlier that *nd* is the dimension of edge Hilbert space about the bipartite graph *BGn*,*<sup>m</sup>*, and the discriminant matrix *D* has *m* singular values, only some of which are non-zero. Space  $H_A$  spanned by { $\langle \alpha_v \rangle$ :  $v \in V$ }, and space  $H_B$  spanned by { $\langle \beta_v \rangle$ :  $e \in E$ }, are *n* – *dimension* and *m* – *dimension* subspaces of  $H^{nd}$ , respectively. Let  $H_{AB}$  be the space spanned by { $\vert \alpha_v \rangle$ :  $v \in V$ }

and  $\{|\beta_e\rangle: e \in E\}$ , and the dimension of  $H_{AB}$  is *rank*( $H_{AB}$ ). Therefore, the dimension of space ( $H_A \cup H_B$ )<sup> $\perp$ </sup> is given by  $nd$  –  $rank(H_{AB})$ , there are  $2m$  eigenvectors in the space  $H_A \cap H_B$ , and  $rank(H_{AB})$  –  $2m$  remaining vectors in the space  $H_A \cup H_B - H_A \cap H_A$ .

Using *A* to left-multiply (30) and *B* to left-multiply (31), We have

$$
AD|\nu_k\rangle = (AA^T)B|\nu_k\rangle = \sigma_k A|\mu_k\rangle,\tag{33}
$$

$$
BDT| \mu_k \rangle = (BBT)A|\mu_k \rangle = \sigma_k B|\nu_k \rangle.
$$
 (34)

As we mentioned before, the action of *A* and *B* preserve the norm of the vectors, and  $|\nu_k\rangle$  and  $|\mu_k\rangle$  are unit vectors, so  $A|\mu_k\rangle$  and  $B|\nu_k\rangle$  also are unit vectors.

**Proposition 3** On space  $(H_A \cup H_B)^{\perp}$ , *W* acts as the identity.

*Proof.* Suppose a vector  $v \in (H_A \cup H_B)^{\perp}$ . Then *v* lies in the space orthogonal to both  $H_A$  and  $H_B$ . Since  $R_i$  reflects a vector orthogonal to  $H_b$ , then  $\nu$  is reflected by both  $R_A$  and  $R_B$ . Then applying a walk operator  $W$  does not change *v*. Hence  $W|v\rangle = |v\rangle$ , and the subspace spanned by such *v* is an invariant subspace.

Observing Proposition 3, we only need to analyze the behavior of *W* in  $H_A \cup H_B$ .

**Theorem 3** The subspace *span*{ $A|\mu_k\rangle$ ,  $B|\nu_k\rangle$ } is invariant under the action *W*.

*Proof.* Suppose we have  $|v\rangle \in H_v^n$  and  $|w\rangle \in H_e^m$ , then we want to analyze the action of  $R_B$  on  $A|v\rangle$  and the action of  $R_A$  on  $B|w\rangle$ . (Since  $A|v\rangle \in H_A$ , the action of  $R_A$  on  $A|v\rangle$  is identity). Since we have

$$
R_{B}A|\nu\rangle = 2BB^{T}A|\nu\rangle - A|\nu\rangle \tag{35}
$$

where the first term of the last line lies in  $H_B$  and the second term in  $H_A$ , and similarly

$$
R_A B|w\rangle = 2AA^T B|w\rangle - B|w\rangle \tag{36}
$$

Hence, we only need to consider the action of *W* on  $A|\mu_k\rangle$  and  $B|\nu_k\rangle$  and that  $A|\mu_k\rangle$  is invariant by  $R_A$  and  $B|\nu_k\rangle$ is invariant by  $R_B$ .

$$
WA|\mu_k\rangle = R_B R_A A|\mu_k\rangle
$$
  
=  $R_B A|\mu_k\rangle$   
=  $2\sigma_k B|\nu_k\rangle - A|\mu_k\rangle$   
=  $(\cos(\theta_k)B|\nu_k\rangle) - (A|\mu_k\rangle - \cos(\theta_k)B|\nu_k\rangle)$  (37)

The first term in the last line is the component of  $A|\mu_k\rangle$  that is along  $B|\nu_k\rangle$  and the second term is the component of  $A|\mu_k\rangle$  that is orthogonal to  $B|\nu_k\rangle$ . So, on  $A|\mu_k\rangle$ ,  $R_A$  is a reflection about  $A|\mu_k\rangle$  (identity in this case), and  $R_B$  is a reflection about  $B|\nu_k\rangle$  { because of the orthogonal component) in the subspace. Similarly, on  $B|\nu_k\rangle$ ,  $R_A$  is a reflection about  $A|\mu_k\rangle$  (because of the orthogonal component), and  $R_B$  is a reflection about  $B|\nu_k\rangle$  (identity) in the subspace.

Next we shall create eigenvectors for *W* with the corresponding eigenvalues. Suppose that

$$
W|k\rangle = \lambda_k|k\rangle \tag{38}
$$

and

$$
|k\rangle = aA|\mu_k\rangle + bB|\nu_k\rangle. \tag{39}
$$

Simply plugging (39) into formulas (38), we obtain the following equation:

$$
W|k\rangle = \lambda_k a A |\mu_k\rangle + \lambda_k b B |\nu_k\rangle. \tag{40}
$$

Then, left-multiplying (39) by *W*, we have

$$
W|k\rangle = W(aA|\mu_k\rangle + bB|\nu_k\rangle)
$$
  
= -(a + 2b\sigma\_k)A|\mu\_k\rangle + [2a\sigma\_k^2 + b(4\sigma\_k - 1)]B|\nu\_k\rangle. (41)

Comparing formulas (40) and (41), we can obtain the following equations:

$$
\lambda_k a = -(a + 2b\sigma_k),\tag{42}
$$

<span id="page-6-7"></span>

**Table 1.** Eigenvalues of *W* obtained from the singular values of *D*, and angles *θk* obtained from the formula  $\sigma_k = \cos \theta_k$ , where  $k = 1, 2, ..., m$ .

$$
\\
$$

$$
\lambda_k b = 2a\sigma_k^2 + b(4\sigma_k - 1). \tag{43}
$$

Concerning unit vectors  $A|\mu_k\rangle$  and  $B|\nu_k\rangle$ , we consider two cases with respect to non-collinearity and collinearity, as follows.

*Case 1*. First, we consider that  $A|\mu_k\rangle$  and  $B|\nu_k\rangle$  are linearly independent.

Using  $\sigma_k = \cos \theta_k$ , we obtain

$$
\lambda_k = e^{\pm 2i\theta_k} \tag{44}
$$

through a series of algebraic operations. Furthermore, we have the corresponding eigenvectors

$$
|k\rangle = \frac{A|\mu_k\rangle - e^{\pm i\theta_k}B|\nu_k\rangle}{\sqrt{2}\sin\theta_k}.
$$
\n(45)

*Case 2.* Then, we consider that  $A|\mu_k\rangle$  and  $B|\nu_k\rangle$  are collinear. However, since  $A|\mu_k\rangle$  is invariant under the action of  $\Pi_A, B|\nu_k\rangle$  also is; and vice versa, since  $B|\nu_k\rangle$  is invariant under  $\Pi_B$ , and  $A|\mu_k\rangle$  also is. Therefore,  $A|\mu_k\rangle$  and  $B|\nu_k\rangle$  are invariant under the action of *W*, and  $A|\mu_k$  are eigenvectors of *W* with eigenvalue 1.

As a consequence, we obtain the following theorem:

**Theorem 4** Let *W* be the unitary evolution operator on *BGn*,*<sup>m</sup>*. Then *W* has eigenvalues 1 and −1 in the one-dimensional subspaces, and eigenvalues  $\lambda_k = e^{\pm 2i\theta_k} \Big( 0 < \theta_k < \frac{\pi}{2} \Big)$  where  $(k = 1, 2, ..., m)$  and the eigenvec- $\langle \mathrm{tors}|k\rangle = \frac{A|\mu_k\rangle - e^{\pm i\theta_k}B\mid \nu_k}{\sqrt{2}\sin\theta_k}$  $|k\rangle = \frac{A|\mu_k\rangle - e^{\pm i\theta_k}B\mid \nu_k\rangle}{\sqrt{2}\sin\theta_k}$  $\frac{B + \nu_{k\ell}}{k}$  in the two-dimensional subspaces Table [1.](#page-6-7)

#### **Discussion**

Quantum walks are one of the elementary techniques of developing quantum algorithms. The development of successful quantum walks on graphs-based algorithms have boosted such areas as element distinctness, searching for a marked element, and graph isomorphism. In addition, the utility of walking on hypergraphs has been probed deeply in several contexts, including natural language parsing, social networks database design, or image segmentation, and so on. Therefore, we put our attention on quantum walks on hypergraphs considering its promising power of inherent parallel computation.

In this paper, we developed a new schema for discrete-time quantum walks on regular uniform hypergraphs using extended Szegedy's walks that naturally quantize classical random walks and yield quadratic speed-up compared to the hitting time of classical random walks. We found the one-to-one correspondence between regular uniform hypergraphs and bipartite graphs. Through the correspondence, we convert the regular uniform hypergraph into its associated bipartite graph on which extended Szegedy's walks take place. In addition, we dealt with the case that the cardinality of the two disjoint sets may be diferent from each other in the bipartite graphs. Furthermore, we delivered spectral properties of the transition matrix, which is the essence of quantum walks, and which has prepared for followup studies.

Our work presents a model for quantum walks on regular uniform hypergraphs, and the model opens the door to quantum walks on hypergraphs. We hope our model can inspire more fruitful results in quantum walks on hypergraphs. Our model provides the foundation for building up quantum algorithms on the strength of quantum walks on hypergraphs. Moreover, the algorithms of quantum walks on hypergraphs will be useful in quantum computation such as quantum walks search, quantized Google's PageRank, and quantum machine learning, based on hypergraphs.

#### **References**

- <span id="page-6-0"></span>1. Bracken, A., Ellinas, D. & Smyrnakis, I. Free-dirac-particle evolution as a quantum random walk. *Phys. Rev. A* **75**, 022322 (2007).
- <span id="page-6-1"></span>2. Childs, A. M. Universal computation by quantum walk. *Phys. review letters* **102**, 180501 (2009).
- <span id="page-6-2"></span>3. Lovett, N. B., Cooper, S., Everitt, M., Trevers, M. & Kendon, V. Universal quantum computation using the discrete-time quantum walk. *Phys. Rev. A* **81**, 042330 (2010).
- <span id="page-6-3"></span>4. Venegas-Andraca, S. E. Quantum walks: a comprehensive review. *Quantum Inf. Process.* **11**, 1015–1106 (2012).
- <span id="page-6-4"></span>5. Aharonov, Y., Davidovich, L. & Zagury, N. Quantum random walks. *Phys. Rev. A* **48**, 1687 (1993).
- <span id="page-6-5"></span>6. Aharonov, D., Ambainis, A., Kempe, J. & Vazirani, U. Quantum walks on graphs. In *Proceedings of the thirty*-*third annual ACM*  symposium on Theory of computing, 50-59 (2001).
- <span id="page-6-6"></span>7. Szegedy, M. Quantum speed-up of markov chain based algorithms. In *Foundations of Computer Science*, *2004*. *Proceedings*. *45th Annual IEEE Symposium on*, 32–41 (2004).
- <span id="page-7-1"></span><span id="page-7-0"></span>8. Nayak, A. & Vishwanath, A. Quantum walk on the line. *arXiv preprint quant*-*ph*/*0010117* (2000).
- <span id="page-7-17"></span><span id="page-7-16"></span><span id="page-7-15"></span><span id="page-7-14"></span><span id="page-7-13"></span><span id="page-7-12"></span><span id="page-7-11"></span><span id="page-7-10"></span><span id="page-7-9"></span><span id="page-7-8"></span><span id="page-7-7"></span><span id="page-7-6"></span><span id="page-7-5"></span><span id="page-7-4"></span><span id="page-7-3"></span><span id="page-7-2"></span>9. Portugal, R., Boettcher, S. & Falkner, S. One-dimensional coinless quantum walks. *Phys. Rev. A* **91**, 052319 (2015).
	- 10. Bednarska, M., Grudka, A., Kurzyński, P., Łuczak, T. & Wójcik, A. Quantum walks on cycles. *Phys. Lett. A* **317**, 21–25 (2003).
	- 11. Melnikov, A. A. & Fedichkin, L. E. Quantum walks of interacting fermions on a cycle graph. *Sci. reports* **6**, 34226 (2016).
	- 12. Moore, C. & Russell, A. Quantum walks on the hypercube. In *International Workshop on Randomization and Approximation Techniques in Computer Science*, 164–178 (2002).
	- 13. Potoček, V., Gábris, A., Kiss, T. & Jex, I. Optimized quantum random-walk search algorithms on the hypercube. *Phys. Rev. A* **79**, 012325 (2009).
	- 14. Chakraborty, S., Novo, L., Ambainis, A. & Omar, Y. Spatial search by quantum walk is optimal for almost all graphs. *Phys. review letters* **116**, 100501 (2016).
	- 15. Wong, T. G. Faster quantum walk search on a weighted graph. *Phys. Rev. A* **92**, 032320 (2015).
	- 16. Krovi, H., Magniez, F., Ozols, M. & Roland, J. Quantum walks can fnd a marked element on any graph. *Algorithmica* **74**, 851–907  $(2016)$
	- 17. Li, D., Mc Gettrick, M., Gao, F., Xu, J. & Wen, Q. Generic quantum walks with memory on regular graphs. *Phys. Rev. A* **93**, 042323 (2016).
	- 18. Ambainis, A. Quantum walk algorithm for element distinctness. *SIAM J. Comput.* **37**, 210–239 (2007).
	- 19. Belovs, A. Learning-graph-based quantum algorithm for k-distinctness. In *Foundations of Computer Science* (*FOCS*), *2012 IEEE 53rd Annual Symposium on*, 207–216 (2012).
	- 20. Magniez, F., Santha, M. & Szegedy, M. Quantum algorithms for the triangle problem. *SIAM J. Comput.* **37**, 413–424 (2007).
	- 21. Lee, T., Magniez, F. & Santha, M. Improved quantum query algorithms for triangle fnding and associativity testing. In *Proceedings of the twenty*-*fourth annual ACM*-*SIAM symposium on Discrete algorithms*, 1486–1502 (2013).
	- 22. Buhrman, H. & Špalek, R. Quantum verifcation of matrix products. In *Proceedings of the seventeenth annual ACM*-*SIAM symposium on Discrete algorithm*, 880–889 (2006).
	- 23. Shenvi, N., Kempe, J. & Whaley, K. B. Quantum random-walk search algorithm. *Phys. Rev. A* **67**, 052307 (2003).
	- 24. Paparo, G. D. & Martin-Delgado, M. Google in a quantum network. *Sci. reports* **2**, 444 (2012).
	- 25. Douglas, B. L. & Wang, J. B. A classical approach to the graph isomorphism problem using quantum walks. *J. Phys. A: Math. Teor.* **41**, 075303 (2008).
	- 26. Wang, H., Wu, J., Yang, X. & Yi, X. A graph isomorphism algorithm using signatures computed via quantum walk search model. *J. Phys. A: Math. Teor.* **48**, 115302 (2015).
	- 27. Kempe, J. Quantum random walks: an introductory overview. *Contemp. Phys.* **44**, 307–327 (2003).
	- 28. Kendon, V. Decoherence in quantum walks–a review. *Math. Struct. Comput. Sci.* **17**, 1169–1220 (2007).
	- 29. Konno, N. Quantum walks. In *Quantum Potential Theory*, 309-452 (Springer, 2008).
	- 30. Venegas-Andraca, S. E. Quantum walks for computer scientists. *Synth. Lect. on Quantum Comput.* **1**, 1–119 (2008).
	- 31. Wang, J. & Manouchehri, K. *Physical implementation of quantum walks* (Springer, 2013).
	- 32. Zhou, D., Huang, J. & Schölkopf, B. Learning with hypergraphs: Clustering, classifcation, and embedding. In *Advances in neural information processing systems*, 1601–1608 (2007).
	- 33. Yu, J., Rui, Y., Tang, Y. Y. & Tao, D. High-order distance-based multiview stochastic learning in image classifcation. *IEEE transactions on cybernetics* **44**, 2431–2442 (2014).
	- 34. Huang, S., Elgammal, A. & Yang, D. On the efect of hyperedge weights on hypergraph learning. *Image Vis. Comput.* **57**, 89–101  $(2017)$
	- 35. Hotho, A., Jäschke, R., Schmitz, C. & Stumme, G. Information retrieval in folksonomies: Search and ranking. *ESWC* **4011**, 411–426  $(2006)$
	- 36. Yu, J., Rui, Y. & Tao, D. Click prediction for web image reranking using multimodal sparse coding. *IEEE Transactions on Image Process.* **23**, 2019–2032 (2014).
	- 37. Zhu, L., Shen, J., Xie, L. & Cheng, Z. Unsupervised visual hashing with semantic assistant for content-based image retrieval. *IEEE Transactions on Knowl. Data Eng.* **29**, 472–486 (2017).
	- 38. Brox, T. Higher order motion models and spectral clustering. In *IEEE Conference on Computer Vision and Pattern Recognition*, 614–621 (2012).
	- 39. Konno, N., Portugal, R., Sato, I. & Segawa, E. Partition-based discrete-time quantum walks. *arXiv preprint arXiv*:*1707*.*07127* (2017).
	- 40. Portugal, R. Establishing the equivalence between szegedy's and coined quantum walks using the staggered model. *Quantum Inf. Process.* **15**, 1387–1409 (2016).
	- 41. Björck, Á. & Golub, G. H. Numerical methods for computing angles between linear subspaces. *Math. Comput.* **27**, 579–594 (1973).

#### <span id="page-7-31"></span><span id="page-7-30"></span><span id="page-7-29"></span><span id="page-7-28"></span><span id="page-7-27"></span><span id="page-7-26"></span><span id="page-7-25"></span><span id="page-7-24"></span><span id="page-7-23"></span><span id="page-7-22"></span><span id="page-7-21"></span><span id="page-7-20"></span><span id="page-7-19"></span><span id="page-7-18"></span>**Acknowledgements**

I would like to thank Juan Xu, Yuan Su and Iwao Sato for helpful discussions. Tis work was supported by the Funding of National Natural Science Foundation of China (Grants No. 61571226 and No. 61701229), and the Natural Science Foundation of Jiangsu Province, China (Grant No. BK20170802).

#### **Author Contributions**

Ying Liu initiated the idea and designed the modle; Ying Liu, Jiabin Yuan, Bojia Duan and Dan Li provided the theoretical proposal and analysis. All authors reviewed the manuscript.

### **Additional Information**

**Competing Interests:** The authors declare no competing interests.

**Publisher's note:** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional afliations.

**Open Access** This article is licensed under a Creative Commons Attribution 4.0 International  $\odot$ License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons license, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons license and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this license, visit [http://creativecommons.org/licenses/by/4.0/.](http://creativecommons.org/licenses/by/4.0/)

 $© The Author(s) 2018$