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Symmetric Quantum Walks on Hamming Graphs and Their Limit Distributions

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Abstract. We study a class of symmetric coined quantum walks on Hamming graphs, where the distance between vertices specifies the transition probability. A special model is the simple quantum walk on the hypercube, which has been discussed in the literature. Eigenvalues of the unitary operator of the quantum walks are zeros of certain self-reciprocal polynomials. We obtain a spectral representation of the wave vector, where our systematic treatment relies on the coin space isomorphic to the state space and the commutative association scheme. The Grover coin is extended to the reflection about a vector in an invariant subspace of the Terwilliger algebra. The limit distributions of several quantum walks are obtained.

Key words: association scheme; hypercube; random walk; self-reciprocal polynomial; spectral representation

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1 Introduction

Random walks on graphs are a typical research topic for finite-state Markov chains. In particular, random walks on cycles and on the hypercube are classical topics, which can be viewed as random walks with the elements of a finite group as their state space. See [7] and references therein.

A simple random walk on the hypercube is a finite Markov chain defined on a state space where each vertex on the hypercube is binary-valued, with transitions occurring only between adjacent vertices. If the dimension of the hypercube is d, the state space can be viewed as a d-digit binary number, with transitions occurring only between numbers that differ by only one digit. In this study, we first discuss more general random walks on finite sets. There are two directions of extension related to this study: one extends the transition probability, allowing transitions to occur between vertices that are not necessarily adjacent. Such random walks are sometimes called long-range random walks. There are several studies on such random walks; see [6] and references there in. The other extends the state space, defined on a state space where each vertex on the hypercube is n-valued. Here, two states that differ at only one vertex are called adjacent. A graph in which adjacency is represented by edges is called a Hamming graph. The Hamming graph is a model of a word of length d consisting of n characters. The number of different characters in two words is the distance in this paper, and is called the Hamming distance. One motivation for considering Hamming graphs is that they are a fundamental object in string processing, including coding theory [2, Chapter 1].

Another motivation for considering Hamming graphs is an interest in group representations and orthogonal polynomials. The transition probability of a simple random walk on the hypercube is invariant under the action of the hyperoctahedral group, and therefore its spectral representation is given by Krawtchouk polynomials, associated with zonal spherical functions [7, Chapter 3]. Hora [11] established that the spectral representation of the transition probability of a class of random walks on the Hamming graph has Krawtchouk polynomial eigenfunctions.

Quantum walks are motivated by search algorithms in quantum computing. While not Markov chains, they are models that incorporate randomness in the quantum mechanical sense. A class of such models is a coined, or discrete-time quantum walk on finite graphs introduced by Aharonov et al. [1]. They discussed quantum walks on cycles, and quantum walks on various finite graphs have been explored in the literature. However, coined quantum walks are harder to analyse than random walks, and explicit results are limited to a few models.

Within this context, quantum walks on the hypercube have been the subject of study by numerous authors since [15], and even the early paper [16], which proposed using quantum walks for search, considered quantum walks on the hypercube. However, to the authors' knowledge, results concerning coined quantum walks on the hypercube are limited to those associated with the simple random walk, and there are no results for general Hamming graphs. While results for continuous-time quantum walks on Hamming graphs exist [4], continuous-time quantum walks are a significantly different model from coined quantum walks, and their analysis is usually not as hard as that of coined quantum walks.

Regarding the methods, for coined quantum walks on the hypercube associated with the simple random walk, [15] and [14] perform direct matrix calculations, while [16] and subsequent papers obtain results through quantum walks on the interval defined by the distance. The latter has the advantage of being able to use the results of the birth-death process, as in [10]. However, it seems difficult to extend these methods to more general quantum walks discussed in this paper.

In this paper, we discuss a class of symmetric coined quantum walks on Hamming graphs, where the distance between vertices specifies the transition probability by using the commutative association scheme. Section 2 introduces random walks on the hypercube and Hamming graphs, on which the class of quantum walks considered in this paper is based. While these results are known, describing them using the commutative association scheme prepares the stage for the next section. Section 3 describes the class of quantum walks considered in this paper. We prepare a coin space isomorphic to the state space and introduce the evolution operator. The coin operator is the reflection about a vector in an invariant subspace of the Terwilliger algebra. We then give the Fourier transform. Section 4 discusses the zeros of self-reciprocal polynomials. We show that these zeros are aligned on the unit circle in the complex plane, and provide an explicit form for special cases. These zeros are eigenvalues of the evolution operator. Section 5 presents the main result of this paper: the spectral representation of the wave vector using the Krawtchouk polynomials. When each vertex is binary, i.e., the hypercube, a particularly explicit form is obtained. In Section 6, as an application of the spectral representation of the wave vector obtained in Section 5, we give limiting distributions for various quantum walks. We also reproduce known results for quantum walks associated with simple random walks on the hypercube as special cases.

2 The class of random walks

We begin with a quick review of the Hamming graph and some related notions. See [3, Chapter III] and [2, Chapter 2] for details. Let a state space $X = \{0, 1, \ldots, n-1\}^d$ where $d, n \geq 2$. Set $\partial(x, y) = |\{i \mid x_i \neq y_i\}|$ for $x = (x_i), y = (y_i) \in X$. The distance ∂ induces a relation $X \times X$ by $(x, y) \in R_i \Leftrightarrow \partial(x, y) = i$, $i \in \{0, 1, \ldots, d\}$. A pair of a finite set and a relation satisfying certain conditions is called an association scheme, and the association scheme $\left(X, \{R_i\}_{i \in \{0,\ldots,d\}}\right)$ introduced here is specifically called the Hamming scheme. The advantage of formulating a problem using an association scheme is that it can reduce the need to perform direct matrix calculations, as will be demonstrated throughout this paper.

An undirected graph (X, R_1) with vertices X and edges R_1 is called a *Hamming graph* $H(d, n)$ (or the *hypercube* if $n = 2$). The adjacency matrix A_i is defined by

$$(A_i)_{x,y} = \begin{cases} 1 & \text{if } (x, y) \in R_i, \\ 0 & \text{if } (x, y) \notin R_i. \end{cases}$$

Let $\mathcal{A}$ be the vector subspace of the matrices $M_X(\mathbb{C})$ spanned by $A_0, A_1, \ldots, A_d$. Here, $\mathcal{A}$ is commutative with the matrix product, and called a Bose–Mesner algebra. Set $\kappa_i = |\{y \in X \mid \partial(x, y) = i\}|$ (the right-hand side being independent of $x \in X$), where κ_1 is the degree of each vertex. Commutative $A_0, A_1, \ldots, A_d$ are simultaneously diagonalised by primitive idempotents $E_0, E_1, \ldots, E_d$ in $\mathcal{A}$ satisfying $E_i E_j = E_i \delta_{i,j}$. Here E_0 denotes the matrix whose entries are all $1/n^d$. The base change determines the coefficients $p_i(j)$ and $q_i(j)$

$$A_i = \sum_{j=0}^{d} p_i(j) E_j, \qquad n^d E_i = \sum_{j=0}^{d} q_i(j) A_j. \tag{2.1}$$

In terms of the Krawtchouk polynomials

$$K_i(j) = \sum_{l=\max\{0,i+j-d\}}^{\min\{i,j\}} (-1)^l (n-1)^{i-l} \binom{j}{l} \binom{d-j}{i-l}, \tag{2.2}$$

we have [3, Section III.2]

$$p_i(j) = q_i(j) = K_i(j), \qquad \text{where} \quad \kappa_i = K_i(0) = (n-1)^i \binom{d}{i}. \tag{2.3}$$

The generating function for the Krawtchouk polynomials is

$$\sum_{l=0}^{d} K_l(j) s^l = (1 + (n-1)s)^{d-j} (1-s)^j.$$

Orthogonality is with respect to the Binomial distribution,

$$\sum_{l=0}^{d} K_i(l) K_j(l) \binom{d}{l} \left(1 - \frac{1}{n}\right)^l \left(\frac{1}{n}\right)^{d-l} = \delta_{i,j} (n-1)^i \binom{d}{i}.$$

Another version of Krawtchouk polynomials with different normalization found in literature is [12, Section 1.10]

$$\frac{K_i(j)}{\kappa_i} = {}_2F_1(-i, -j; -d; n/(n-1)),$$

which are the zonal spherical functions of the permutation group $S_n \wr S_d$ on X.

Hora [11] discussed random walks on the Hamming graph $H(d, n)$ with transition probability matrix P. He assumed a spatial symmetry of P that it is constant on each orbit R_i:

$$\partial(x, y) = \partial(x', y') \quad \Rightarrow \quad (P)_{x,y} = (P)_{x',y'} \tag{2.4}$$

or equivalently that P belongs to Bose–Mesner algebra $\mathcal{A}$.

Under this assumption, the transition probability takes the form of

$$P = \sum_{i=0}^{d} \frac{w_i}{\kappa_i} A_i, \qquad \text{where} \quad w_i \geq 0, \ \sum_{i=0}^{d} w_i = 1. \tag{2.5}$$

Let $P_t(h)$, $t \in \mathbb{N} := \{0,1,\dots\}$ denote the t-step transition probability $\left(P^t\right)_{x,y}$ for $(x,y) \in R_h$. Hora [11] established a spectral representation

$$P_t(h) = \frac{1}{n^d} \sum_{i=0}^{d} \rho_i^t K_i(h), \qquad h \in \{0,1,\dots,d\} \tag{2.6}$$

with eigenvalues

$$\rho_i = \sum_{j=0}^{d} \frac{w_j}{\kappa_j} K_j(i) = \sum_{j=0}^{d} \frac{w_j}{\kappa_i} K_i(j), \qquad i \in \{0,1,\dots,d\}. \tag{2.7}$$

This follows immediately. Since

$$P = \sum_{i=0}^{d} \frac{w_i}{\kappa_i} \sum_{j=0}^{d} p_i(j) E_j = \sum_{j=0}^{d} \rho_j E_j$$

holds by (2.1), we have

$$P^t = \sum_{i=0}^{d} \rho_i^t E_i = \frac{1}{n^d} \sum_{i=0}^{d} \sum_{j=0}^{d} \rho_i^t q_i(j) A_j = \frac{1}{n^d} \sum_{i=0}^{d} \sum_{j=0}^{d} \rho_i^t K_i(j) A_j,$$

where the first and last equalities follow from $E_i E_j = E_i \delta_{i,j}$ and (2.3), respectively. We note that $\rho_0 = 1$ and

$$-\frac{1}{n-1} \le \rho_i \le 1, \qquad i \in \{1,\dots,d\}. \tag{2.8}$$

For the lower bound in (2.8), see [8, Theorem 1]. If a random walk is irreducible and aperiodic -1 is not an eigenvalue. Since the transition probability (2.5) is symmetric, the stationary distribution is uniform. Hora [11] gave a detailed treatment of the cut-off phenomenon of a simple random walk ($w_i = \delta_{i,1}$). Collevechio and Griffiths [6] obtained (2.6) for a broad class of random walks on the hypercube, i.e., $H(d,2)$, which contains the class satisfying assumption (2.4).

We consider a random walk starting from a state of X. Without loss of generality, let the state be 0. In the standard basis of the vector space $\mathbb{C}^X$, the element corresponding to 0 is denoted by e_0. Then,

$$P_{0,x} = \sum_{i=0}^{d} \frac{w_i}{\kappa_i} (A_i)_{0,x} = \sum_{i=0}^{d} \frac{w_i}{\kappa_i} (A_i e_0)_x = \frac{w_{|x|}}{\kappa_{|x|}}, \qquad |x| := \partial(0,x), \tag{2.9}$$

where $\{(A_i e_0)_x : x \in X\}$ is the standard basis of a T-invariant subspace, called the principal T-module, of the Terwilliger algebra $T = \langle \mathcal{A}, \mathcal{A}^* \rangle$ with respect to e_0, where $\mathcal{A}^* = \mathcal{A}^*(e_0)$ is the dual Bose–Mesner algebra of $\mathcal{A}$. Furthermore, since $P \in \mathcal{A}$ by assumption (2.4), we can see that the state of the random walk is contained in the principal T-module at any given time. For the Terwilliger algebra, see [2, Section 2.6].

Remark 2.1. The representation of the eigenvalues (2.7) is known in classic Markov chain theory [8]. Suppose we have a Markov chain $\{Z_t \mid t \ge 0\}$ whose stationary distribution is a binomial distribution of length d and parameter $1 - 1/n$, and the transition probability is

$$P_{0,z} = \binom{d}{z} \left(1 - \frac{1}{n}\right)^z \left(\frac{1}{n}\right)^{d-z} \sum_{i=0}^{d} \rho_i K_i(z).$$

Then, ρ_i has the representation (2.7). This Markov chain $\{Z_t \mid t \ge 0\}$ coincides with that of the distance $|x|$ with the transition probability (2.5) and starting from 0.

Some examples of random walks on $H(d,n)$ satisfying assumption (2.4) are the following.

Example 2.2 (the simple random walk)**.** A walker at x moves to a neighbour $y \in X$ satisfying $\partial(x,y)=1$ with equal probability,

$$w_i = \delta_{i,1}, \qquad \rho_i = 1 - \frac{ni}{(n-1)d}, \qquad i \in \{0,1,\ldots,d\}.$$

This random walk is irreducible and periodic if $n=2$ and aperiodic otherwise.

Example 2.3 (the independent random walk)**.** A walker at $x \in X$ moves to any $y \in X$ with equal probability,

$$w_i = \frac{\kappa_i}{n^d} = \binom{d}{i}\frac{(n-1)^i}{n^d}, \qquad \rho_i = \delta_{i,0}, \qquad i \in \{0,1,\ldots,d\}.$$

This random walk is irreducible and aperiodic. This random walk mixes in exactly one step.

Example 2.4 (the non-local random walk with cardinality $m \in \{2,\ldots,d\}$)**.** A walker at $x \in X$ moves to $y \in X$ satisfying $\partial(x,y)=m$ with equal probability,

$$w_i = \delta_{i,m}, \qquad \rho_i = \frac{K_m(i)}{\kappa_m}, \qquad i \in \{0,1,\ldots,d\}.$$

If $n=2$, this random walk is periodic, and irreducible if m is odd and reducible otherwise. If $n \geq 3$, this random walk is irreducible and aperiodic.

Example 2.5 (the mixture of i.i.d. updates for each coordinate)**.** The cardinality $i \in \{0,1,\ldots,d\}$ is drawn from the binomial distribution of random parameter $\alpha \in (0,1)$ following some mixing measure. A walker at $x \in X$ moves to $y \in X$ satisfying $\partial(x,y)=i$ with equal probability. Collevechio and Griffiths [6] discussed the model of $n=2$.

$$w_i = \binom{d}{i}\alpha^i(1-\alpha)^{d-i}, \qquad \rho_i = \left(1 - \frac{n\alpha}{n-1}\right)^i, \qquad i \in \{0,1,\ldots,d\}.$$

This random walk is irreducible and aperiodic.

3 The class of quantum walks

Let $X = \{0,1,\ldots,n-1\}^d$ be position and coin space, respectively, equipped with Hilbert spaces $\mathcal{H}_P$ and $\mathcal{H}_C$ with bases $\{|x\rangle\}_{x\in X}$ and $\{|y\rangle\}_{y\in X}$. The dual bases are denoted by $\{\langle x|\}_{x\in X}$ and $\{\langle y|\}_{y\in X}$. A quantum state at step $t \in \mathbb{N}$ is represented as

$$|\Psi(t)\rangle = \sum_{y\in X}\sum_{x\in X}\psi_{y,x}(t)|y,x\rangle, \qquad |y,x\rangle = |y\rangle \otimes |x\rangle,$$

where $\{\psi_{y,x}(t)\} \in \mathbb{C}^{X\times X}$ is called the wave vector. The probability that we observe the quantum walker at position $x \in X$ after t-steps is

$$P_t(x) = \sum_{y\in X}|\psi_{y,x}(t)|^2.$$

The evolution operator for one step of the quantum walk is

$$U = S \circ (C \otimes I), \tag{3.1}$$

where $C=\sum_{y,y'\in X} C_{y,y'}|y\rangle\langle y'|$ is called a coin operator in $\mathcal{H}_C$, I is the identity in $\mathcal{H}_P$, and S is the shift operator defined by

$$S=\sum_{y\in X}\sum_{x\in X}|y,x\oplus y\rangle\langle y,x|.$$

Here, $x\oplus y$ is the component-wise sum of d-dimensional vectors x and y of modulo n. This shift operator reduces to the standard shift operator in quantum walks on a hypercube associated with the simple random walk used in [14, 15, 16], when $n=2$ and y is an element of the standard basis of the vector space $\mathbb{C}^d$. Furthermore, $S^n=I$. Thus, S is a natural extension of the standard shift operator. Applying U, we obtain the one-step transition of components of the wave vector:

$$\begin{aligned}\psi_{y,x}(t+1)&=\sum_{y'\in X}\sum_{x'\in X}U_{y,x;y',x'}\psi_{y',x'}(t)\\&=\sum_{y'\in X}C_{y,y'}\psi_{y',x\oplus(n-1)y}(t),\qquad x,y\in X,\ t\geq 0,\end{aligned}\tag{3.2}$$

where

$$\oplus(n-1)y=\overbrace{\oplus y\oplus y\oplus y\oplus\cdots\oplus y}^{(n-1)\text{-times}}$$

and

$$U=\sum_{y\in X}\sum_{y'\in X}\sum_{x\in X}\sum_{x'\in X}U_{y,x;y',x'}|y,x\rangle\langle y',x'|.$$

We consider a class of coined quantum walks on Hamming graph $H(d,n)$ stimulated by random walks discussed in the previous section. As for the coin operator, we take a common choice, so called Szegedy's walk [17], associated with the random walk determined by the transition probability (2.5). Namely, (2.9) determines

$$C_{y,y'}=2\sqrt{P_{0,y}P_{0,y'}}-\delta_{y,y'}=2\sqrt{\frac{w_{|y|}}{\kappa_{|y|}}\frac{w_{|y'|}}{\kappa_{|y'|}}}-\delta_{y,y'},\qquad y,y'\in X.\tag{3.3}$$

We can confirm that C is orthogonal. This coin operator reduces to the standard d-dimensional Grover coin in quantum walks on a hypercube associated with the simple random walk used in [15, 16], when $n=2$ and $w_i=\delta_{i,1}$. Since

$$\sum_{y\in X}\sum_{y'\in X}\sqrt{\frac{w_{|y|}}{\kappa_{|y|}}\frac{w_{|y'|}}{\kappa_{|y'|}}}|y\rangle\langle y'|$$

is a projection operator to the principal T-module, C is a reflection about a unit vector in the principal T-module with respect to 0. We set the initial state

$$\psi_{y,x}(0)=\delta_{x,0}\sqrt{\frac{w_{|y|}}{\kappa_{|y|}}},\qquad x,y\in X,\tag{3.4}$$

which means that the quantum walk starts from position 0 with law (2.9) in the coin space

$$|\psi_{y,x}(0)|^2=\delta_{x,0}\frac{w_{|y|}}{\kappa_{|y|}},\qquad x,y\in X,$$

where $\sum_{y\in X}\sum_{x\in X}|\psi_{y,x}(0)|^2=1$, since $\sum_{y\in X} w_{|y|}/\kappa_{|y|}=1$. Moreover, the initial coin

$$\sum_{y\in X}\sqrt{\frac{w_{|y|}}{\kappa_{|y|}}}|y\rangle=\sum_{y\in X}\sum_{i=0}^{d}\sqrt{\frac{w_i}{\kappa_i}}(A_ie_0)_y|y\rangle$$

is the unit vector in the principal T-module. An observation here is that $\{\psi_{y,x}(t)\}\in\mathbb{R}^{X\times X}$ for all $t\in\mathbb{N}$.

To solve (3.2), we employ the Fourier transform in the position space, which is standard in analyses of quantum walks on graphs [1],

$$\tilde{\psi}_{y,\xi}(t)=\frac{1}{\sqrt{n^d}}\sum_{x\in X}\zeta^{\xi\cdot x}\psi_{y,x}(t)$$

and the inverse transform

$$\psi_{y,x}(t)=\frac{1}{\sqrt{n^d}}\sum_{\xi\in X}\zeta^{-\xi\cdot x}\tilde{\psi}_{y,\xi}(t),$$

where $\zeta\equiv \mathrm{e}^{2\pi\sqrt{-1}/n}$, $\xi\cdot x=\sum_{i=1}^d\xi_ix_i$. We have

$$\begin{aligned}\tilde{\psi}_{y,\xi}(t+1)&=\frac{1}{\sqrt{n^d}}\sum_{y'\in X}\sum_{x\in X}\zeta^{\xi\cdot x}C_{y,y'}\psi_{y',x\oplus(n-1)y}(t)=\frac{1}{\sqrt{n^d}}\sum_{y'\in X}\sum_{x'\in X}\zeta^{\xi\cdot(x'\oplus y)}C_{y,y'}\psi_{y',x'}(t)\\&=\zeta^{\xi\cdot y}\sum_{y'\in X}C_{y,y'}\tilde{\psi}_{y',\xi}(t),\qquad y,\xi\in X,\ t\geq 0,\end{aligned}\tag{3.5}$$

where in the second equality we set $x'=x\oplus(n-1)y$ and used $\zeta^{\xi\cdot x}=\zeta^{\xi\cdot(x\oplus ny)}=\zeta^{\xi\cdot(x'\oplus y)}$, since $\zeta^{n\xi\cdot y}=1$. The advantage of working in the ξ-coordinate is that (3.5) becomes a system of equations that is separated with respect to each ξ. Although (3.5) is not separated in the coin space, it can be solved, as we will see in Section 5.

4 Zeros of a self-reciprocal polynomial

A polynomial $p_n(z)$ of degree n is self-reciprocal if $p_n(z)=p_n^*(z)$, $p_n^*(z):=z^n\overline{p_n(1/\bar{z})}$. The distribution of the zeros of such a polynomial are interesting in their own right. At the end of this section, we will see that the zeros are the eigenvalues of the evolution operator of the quantum walks. The following result is anticipated because U is unitary.

Lemma 4.1. *For constant $\rho\in[-1/(n-1),1]$, $n\geq 2$, all of the zeros of polynomial*

$$z^n+2\rho\sum_{i=1}^{n-1}z^i+1,\qquad z\in\mathbb{C}\tag{4.1}$$

are on the unit circle, namely, $\{z\in\mathbb{C}\mid |z|=1\}$.

Proof. Suppose $1\geq\rho>0$. The polynomial (4.1) is self-reciprocal and represented as

$$p_n(z)=z^n+2\rho\sum_{i=1}^{n-1}z^i+1=zq_{n-1}(z)+q_{n-1}^*(z),$$

where $q_{n-1}(z)=z^{n-1}+\rho\sum_{i=0}^{n-2}z^i$. According to Chen [5, Theorem 1], all the zeros of $p_n(z)$ lie on the unit circle if all the zeros of $q_{n-1}(z)$ are in or on the unit circle. By the Eneström–Kakeya theorem, all the zeros of $q_{n-1}(z)$ lie in or on the unit circle since $1\geq\rho>0$. Therefore, the assertion holds. If $\rho = 0$, the zeros are the n-th roots of -1. Finally, suppose $-1/(n-1) \le \rho < 0$. Theorem 1 of Lakatos and Losonczi [13] says that all the zeros of a self-reciprocal polynomial $\sum_{i=0}^{n} a_i z^i$, $a_i = a_{n-i}$, $i \in \{0, \dots, n\}$ are on the unit circle if

$$|a_0| \ge \frac{1}{2} \sum_{i=1}^{n-1} |a_i|,$$

and $p_n(z)$ satisfies this if $-1/(n-1) \le \rho \le 1/(n-1)$. ■

In the following, we assume n is prime, namely, $\zeta^k = \mathrm{e}^{2\pi\sqrt{-1}k/n}$, $k \in \{1, 2, \dots, n-1\}$ are the primitive roots of unity. This assumption makes following expressions explicit. We collect some properties of the zeros of the polynomial (4.1).

Proposition 4.2. *Assume n is a prime. If unity is a zero of the polynomial (4.1), then $\rho = -1/(n-1)$, and if a primitive root of unity is a zero, then $\rho = 1$.*

Proof. The first assertion follows immediately. The second assertion follows by

$$\sum_{i=1}^{n-1} \zeta^{ki} = \sum_{i=0}^{n-1} \zeta^{ki} - 1 = \frac{1 - \zeta^{kn}}{1 - \zeta^k} - 1 = -1, \qquad k \in \{1, \dots, n-1\},$$

where $\zeta \equiv \mathrm{e}^{2\pi\sqrt{-1}/n}$. ■

Proposition 4.3. *For prime n (≥ 3), the zeros of the polynomial (4.1) are -1 and the following:*

(*i*) *if $\rho = 1$, the primitive roots of unity $\zeta^k = \mathrm{e}^{2\pi\sqrt{-1}k/n}$, $k \in \{1, 2, \dots, n-1\}$;*

(*ii*) *if $\rho = 0$, $-\zeta^k$, $k \in \{1, 2, \dots, n-1\}$;*

(*iii*) *if $\rho = -1/(n-1)$, unity, and those on the unit circle except for ± 1 and the primitive roots of unity if $n \ge 5$.*

Proof. (*i*) The polynomial factors as $(z+1)\big(z^{n-1} + z^{n-2} + \cdots + z + 1\big)$. Since the second factor is the n-th cyclotomic polynomial, the zeros are the n-th primitive roots of unity. (*ii*) Similar to (*i*). (*iii*) The polynomial factors as

$$(z-1)^2(z+1)\left\{\sum_{i=1}^{n-2} \left\lceil \frac{i}{2} \right\rceil \left(n - 2\left\lfloor \frac{i}{2} \right\rfloor - 1\right) \frac{z^{n-i-2}}{n-1}\right\}.$$

The last factor is a polynomial of order $n-3$. The zeros of the polynomial are on the unit circle by Lemma 4.1, and not the primitive roots of unity by Proposition 4.2 ■

In the following part of this paper, the zeros of the polynomial (4.1) with replacing z by $-z$:

$$(-z)^n + 2\rho \sum_{i=1}^{n-1} (-z)^i + 1, \qquad z \in \mathbb{C} \tag{4.2}$$

appear.

Remark 4.4. If $n = 2$, (4.2) gives $2\rho = z + 1/z$ and the real part of the zeros is ρ, since a zero is on the unit circle. The mapping $z \mapsto z + 1/z$ is a conformal map known as the Joukowsky transform. The Joukowsky transform maps the unit circle to the real interval $[-2, 2]$. For a prime $n \ge 3$, we have

$$2\rho = \frac{1}{\sum_{i=1}^{n-1} z^i} + \frac{1}{\sum_{i=1}^{n-1} z^{-i}}.$$

The mapping $z \mapsto 1/\sum_{i=1}^{n-1} z^i + 1/\sum_{i=1}^{n-1} z^{-i}$ is also a conformal map which maps the unit circle to the real interval. The argument θ of a zero satisfies

$$2\rho = 1 + \frac{\cos\theta - \cos(n\theta)}{1 - \cos\{(n-1)\theta\}}.$$

Proposition 4.5. *Consider a random walk on a Hamming graph $H(d,n)$, $d \geq 2$ and prime n satisfying assumption (2.4). Any eigenvalue of the evolution operator (3.1) of the quantum walk with coin operator (3.3) is a zero of the polynomial (4.2) with $\rho = \rho_{|\xi|}$ for some $\xi \in X$.*

We prepare a lemma to prove Proposition 4.5. It provides the Fourier transform of functions of $|z| = \partial(0,z)$ by the characters of the direct product of the cyclic groups of order n.

Lemma 4.6. *For any function $f\colon \{0,1,\dots,d\} \to \mathbb{C}$ and prime n, we have*

$$\sum_{z\in X} \zeta^{k\xi\cdot z} f(|z|) = \sum_{j=0}^{d} K_j(|\xi|) f(j), \qquad \xi \in X, \quad k \in \{1,\dots,n-1\} \tag{4.3}$$

and

$$\sum_{\xi\in X} \zeta^{-k\xi\cdot z} f(|\xi|) = \sum_{j=0}^{d} K_j(|z|) f(j), \qquad z \in X, \quad k \in \{1,\dots,n-1\}, \tag{4.4}$$

where $\zeta \equiv \mathrm{e}^{2\pi\sqrt{-1}/n}$.

Proof. Since $\zeta^{jn} = 1$ for $j \in \mathbb{Z}$,

$$\sum_{l=1}^{n-1} \zeta^{kjl} = \frac{1-\zeta^{kjn}}{1-\zeta^{kj}} - 1 = -1, \qquad j,k \in \{1,\dots,n-1\}, \tag{4.5}$$

where $\zeta^{kj} = \mathrm{e}^{2\pi\sqrt{-1}kj/n} \neq 1$ since n is prime. Without loss of generality, we assume $\xi_1,\dots,\xi_{|\xi|} > 0$ and $\xi_{|\xi|+1} = \cdots = \xi_d = 0$. Fix $|z| \in \{0,\dots,d\}$, $l \in \{0,\dots,\min\{|\xi|,|z|\}\}$, and suppose $z_{i_1},\dots,z_{i_l} > 0$, $\{i_1,\dots,i_l\} \in \{1,\dots,|\xi|\}$ and $z_{i_{l+1}},\dots,z_{i_{|z|}} > 0$, $\{i_{l+1},\dots,i_{|z|}\} \in \{|\xi|+1,\dots,d\}$. The contribution of such $z_1,\dots,z_d$ to the left-hand side of (4.3) is $f(|z|)$ times

$$\binom{|\xi|}{l}\binom{d-|\xi|}{|z|-l} \prod_{j=1}^{l} \left(\sum_{z_{i_j}=1}^{n-1} \zeta^{k\xi_j z_{i_j}} \right) (n-1)^{|z|-l} = \binom{|\xi|}{l}\binom{d-|\xi|}{|z|-l} (-1)^l (n-1)^{|z|-l}, \tag{4.6}$$

where we used (4.5). Summing up (4.6) in l yields

$$\sum_{l=\max\{0,|z|+|\xi|-d\}}^{\min\{|\xi|,|z|\}} \binom{|\xi|}{l}\binom{d-|\xi|}{|z|-l} (-1)^l (n-1)^{|z|-l} = K_{|z|}(|\xi|). \tag{4.7}$$

Summation of (4.7) in $|z|$ is the right-hand side of (4.3). We can confirm (4.4) in the same manner. ■

Remark 4.7. Consider the map $\eta_j\colon x_j \mapsto \zeta^{\xi_j x_j}$, where $\eta(x) = \prod_{j=1}^{d} \eta_j(x_j) = \zeta^{\xi\cdot x}$ comprises the character group of the direct product of the cyclic group of order n. If we set $f(z) = \delta_{z,j}$ and $k=1$, then (4.3) reduces to the relation

$$\eta(X_j) = \sum_{x\in X\colon |x|=j} \eta(x) = \sum_{x\in X\colon |x|=j} \zeta^{\xi\cdot x} = K_j(|\xi|), \tag{4.8}$$

where $X_j = \sum_{x\in X\colon |x|=j} x$ is an element of a Schur-ring over X. This relation is Proposition 2.2 in Section III, [3] and used to establish (2.3). However, note that (4.8) holds for any $n \geq 2$, while n should be prime for (4.3) if $k \in \{2,\dots,n-1\}$.

An immediate consequence for (2.7) is the following.

Corollary 4.8. *We have*

$$\rho_{|\xi|} = \sum_{z\in X} \zeta^{k\xi\cdot z} \frac{w_{|z|}}{\kappa_{|z|}}, \qquad \xi \in X,\ k \in \{1,\dots,n-1\}. \tag{4.9}$$

Proof of Proposition 4.5. Let $|v\rangle = \sum_{y\in X}\sum_{x\in X} v_{y,x}|y,x\rangle$ and μ be an eigenvector and the eigenvalue of the evolution operator (3.1), respectively. That is, we have

$$\sum_{y'\in x}\sum_{x'\in X} U_{y,x;y',x'} v_{y',x'} = \sum_{y'\in X} C_{y,y'} v_{y',x\oplus(n-1)y} = \mu v_{y,x}. \tag{4.10}$$

Let

$$u_{y,\xi} = \sqrt{\frac{w_{|y|}}{n^d \kappa_{|y|}}} \sum_{x\in X} \zeta^{\xi\cdot x} v_{y,x}$$

for some $\xi \in X$. We consider the following two cases.

Case 1. Suppose we can take ξ such that $\sum_{y\in X} u_{y,\xi} \neq 0$. By the same argument as obtaining (3.5) from (3.2), we recast the right equality of (4.10) into

$$\mu\zeta^{-\xi\cdot y} u_{y,\xi} = -u_{y,\xi} + 2\frac{w_{|y|}}{\kappa_{|y|}} \sum_{y'\in X} u_{y',\xi}. \tag{4.11}$$

Summing up both sides of (4.11) in $y \in X$ gives

$$\mu \sum_{y\in X} \zeta^{-y\cdot\xi} u_{y,\xi} = -\sum_{y\in X} u_{y,\xi} + 2\sum_{y\in X} \frac{w_{|y|}}{\kappa_{|w|}} \sum_{y'\in X} u_{y',\xi} = \sum_{y\in X} u_{y,\xi}, \tag{4.12}$$

because $\sum_{y\in X} w_{|y|}/\kappa_{|y|} = 1$. Multiplying by $\zeta^{ky\cdot\xi}$, $k \in \{1,\dots,n-1\}$ and summing up both sides of (4.11) gives

$$\mu \sum_{y\in X} \zeta^{(k-1)y\cdot\xi} u_{y,\xi} = -\sum_{y\in X} \zeta^{ky\cdot\xi} u_{y,\xi} + 2\rho_{|\xi|} \sum_{y\in X} u_{y,\xi}, \tag{4.13}$$

where we used (4.9). Since $\zeta^{nz\cdot\xi} = 1$, recursive use of (4.13) gives

$$\begin{aligned}
\mu^n \sum_{y\in X} u_{y,\xi} &= -\mu^{n-1} \sum_{y\in X} \zeta^{y\cdot\xi} u_{y,\xi} + 2\mu^{n-1}\rho_{|\xi|} \sum_{y\in X} u_{y,\xi} \\
&= \mu^{n-2} \sum_{y\in X} \zeta^{2y\cdot\xi} u_{y,\xi} - 2\mu^{n-2}\rho_{|\xi|} \sum_{y\in X} u_{y,\xi} + 2\mu^{n-1}\rho_{|\xi|} \sum_{y\in X} u_{y,\xi} \\
&= (-1)^{n-1}\mu \sum_{y\in X} \zeta^{(n-1)y\cdot\xi} u_{y,\xi} + 2\rho_{|\xi|} \sum_{j=1}^{n-1} (-1)^{n-j-1}\mu^j \sum_{y\in X} u_{y,\xi} \\
&= (-1)^{n-1} \sum_{y\in X} u_{y,\xi} + 2\rho_{|\xi|} \sum_{j=1}^{n-1} (-1)^{n-j-1}\mu^j \sum_{y\in X} u_{y,\xi},
\end{aligned}$$

where (4.12) is used in the last equality. Since $\sum_{y\in X} u_{y,\xi}$ is non-zero, we have

$$(-\mu)^n + 2\rho_{|\xi|} \sum_{j=1}^{n-1} (-\mu)^j + 1 = 0,$$

which shows that μ is a zero of the polynomial (4.2).

Case 2. Suppose $\sum_{y\in X} u_{y,\xi} = 0$ for all $\xi \in X$. Since

$$\sum_{y\in X}\sqrt{\frac{w_{|y|}}{\kappa_{|y|}}}v_{y,x} = \sum_{y\in X}\sum_{\xi\in X}\zeta^{-\xi\cdot x}u_{y,\xi}\sum_{\xi\in X}\zeta^{-\xi\cdot x}\sum_{y\in X}u_{y,\xi} = 0,$$

the vector $\sum_{y\in X} v_{y,x}|y\rangle$ is in the orthogonal complement of the principal T-module, and (4.10) reduces to $v_{y,x\oplus(n-1)y} = -\mu v_{y,x}$. Therefore, we have

$$(-\mu)^n v_{y,x} = (-\mu)^{n-1}v_{y,x\oplus(n-1)y} = \cdots = v_{y,x\oplus n(n-1)y} = v_{y,x}$$

for all $x, y \in X$. If $n = 2$, $\mu = 1$ or -1, which are the zeros of the polynomial (4.2) with $\rho = -1$ and $\rho = 1$, respectively. If $n \geq 3$, $-\mu$ is an n-th root of unity, and by Proposition 4.2, it is a zero of the polynomial (4.2) with $\rho = -1/(n-1)$ or $\rho = 1$. ■

5 Spectral representation of wave vectors

The following spectral representations of the wave vector of the quantum walks on Hamming graphs are the main results of this paper. In this section, we establish them.

Theorem 5.1 (spectral representation of wave vector)**.** *Consider a random walk on a Hamming graph $H(d,n)$, $d \geq 2$ and prime n satisfying assumption* (2.4) *with the eigenvalues $-1/(n-1) < \rho_j < 1$, $j \in \{1,\dots,d\}$. Let $\mu_j^{(1)},\dots,\mu_j^{(n)}$ be the zeros of the polynomial* (4.2) *with $\rho = \rho_j$, $j \in \{1,\dots,d\}$ and assume they are distinct for each j. The wave vector of the quantum walk with coin operator* (3.3) *and the initial state* (3.4) *is represented as*

$$\psi_{y,x}(t) = \frac{1}{n^d}\sqrt{\frac{w_{|y|}}{\kappa_{|y|}}}\sum_{k=0}^{n-1}\sum_{l=0}^{n-1}\frac{\zeta^{lk}}{n} \times\left\{1+\sum_{j=1}^{d}K_j(|x\oplus ly|)\left[\left(-\zeta^{-k}\right)^t\left(1-\sum_{i=1}^{n}\frac{2c_j^{(i)}}{1+\zeta^k\mu_j^{(i)}}\right)+\sum_{i=1}^{n}\frac{2c_j^{(i)}\left(\mu_j^{(i)}\right)^t}{1+\zeta^k\mu_j^{(i)}}\right]\right\},$$

where

$$c_j^{(i)} = \frac{\left(\mu_j^{(i)}\right)^n + (1-\rho_j)\left(\mu_j^{(i)}\right)^{n-1} - \rho_j(-1)^n}{n\left(\mu_j^{(i)}\right)^n + [n-2\rho_j(n-1)]\left(\mu_j^{(i)}\right)^{n-1} - 2\rho_j(-1)^n\sum_{k=0}^{n-2}\left(-\mu_j^{(i)}\right)^k} \tag{5.1}$$

and $\zeta \equiv \mathrm{e}^{2\pi\sqrt{-1}/n}$.

We need the assumptions on the eigenvalues and zeros of the polynomial (4.2) to display the expression in the concise form. For Hamming graphs $H(d,2)$, $d \geq 2$ (or the hypercube of dimension d), we can obtain more explicit results without such assumptions. This is because the algebraic forms of the zeros of the quadratic polynomial (4.2) are available. In this sense, we cannot expect to have general and explicit expressions if $n \geq 7$. This is because we need zeros of the polynomial of degree $(n-1)$ (the unity is always a root of (4.2)), and if $n \geq 7$, we need explicit expressions of the roots of the polynomial of degree larger than 5.

Corollary 5.2 (spectral representation of wave vector, $n = 2$)**.** *Consider a random walk on the Hamming graph $H(d,2)$, $d \geq 2$ satisfying assumption* (2.4)*. The wave vector of the quantum walks with coin operator* (3.3) *and the initial state* (3.4) *is represented as*

$$\psi_{y,x}(t) = \frac{1}{2^d}\sqrt{\frac{w_{|y|}}{\kappa_{|y|}}}\left\{1+\frac{1}{2}\sum_{j:\,|\rho_j|<1}\left[\frac{\left(\mu_j^+\right)^t}{1-\rho_j\mu_j^+}+\frac{\left(\mu_j^-\right)^t}{1-\rho_j\mu_j^-}\right]K_j(|x|)\right.$$

$$- \frac{1}{2} \sum_{j:\ |\rho_j|<1} \left[\frac{\left(\mu_j^+\right)^{t+1}}{1-\rho_j\mu_j^+} + \frac{\left(\mu_j^-\right)^{t+1}}{1-\rho_j\mu_j^-} \right] K_j(|x \oplus y|)$$
$$+ \sum_{j>0:\ \rho_j=1} [(1-t)K_j(|x|) + tK_j(|x \oplus y|)]$$
$$\left. + \sum_{j>0:\ \rho_j=-1} (-1)^t [(1-t)K_j(|x|) - tK_j(|x \oplus y|)] \right\} \tag{5.2}$$

where

$$\mu_j^\pm = \rho_j \pm \sqrt{-1}\sqrt{1-\rho_j^2}, \qquad j \in \{0,\dots,d\},$$

and (ρ_j) *are the eigenvalues of the random walk* (2.7).

We prepare a proposition to prove Theorem 5.1.

Proposition 5.3. *Fix* $\xi \in X \setminus \{0\}$ *and assume* $-1/(n-1) < \rho_{|\xi|} < 1$ *for prime* n. *Let* $\mu_{|\xi|}^{(1)}, \dots, \mu_{|\xi|}^{(n)}$ *be the zeros of the polynomial* (4.2). *If they are distinct, the solution of system* (3.5) *is represented as*

$$\tilde{\psi}_{y,\xi}(t) = \left[\left(-\zeta^{-y\cdot\xi}\right)^t \left(1 - \sum_{i=1}^n \frac{2c_{|\xi|}^{(i)}}{1+\zeta^{y\cdot\xi}\mu_{|\xi|}^{(i)}} \right) + \sum_{i=1}^n \frac{2c_{|\xi|}^{(i)}\left(\mu_{|\xi|}^{(i)}\right)^t}{1+\zeta^{y\cdot\xi}\mu_{|\xi|}^{(i)}} \right] \tilde{\psi}_{y,\xi}(0), \qquad t \geq 0. \tag{5.3}$$

In addition, $\tilde{\psi}_{y,0}(t) = \tilde{\psi}_{y,0}(0)$, $t \geq 0$.

Proof. Let

$$\phi_{y,\xi}(t) = \sqrt{\frac{w_{|y|}}{\kappa_{|y|}}}\tilde{\psi}_{y,\xi}(t).$$

Then, we recast (3.5) into

$$\zeta^{-\xi\cdot y}\phi_{y,\xi}(t+1) = -\phi_{y,\xi}(t) + 2\frac{w_{|y|}}{\kappa_{|y|}} \sum_{y'\in X} \phi_{y',\xi}(t), \qquad t \geq 0 \tag{5.4}$$

with the initial condition

$$\phi_{y,\xi}(0) = \frac{w_{|y|}}{\kappa_{|y|}} \frac{1}{\sqrt{n^d}}.$$

Summing up both sides of (5.4) in $y \in X$ gives

$$\sum_{y\in X} \zeta^{-y\cdot\xi}\phi_{y,\xi}(t+1) = -\sum_{y\in X}\phi_{y,\xi}(t) + 2\sum_{y\in X}\frac{w_{|y|}}{\kappa_{|y|}}\sum_{y'\in X}\phi_{y',\xi}(t) = \sum_{y\in X}\phi_{y,\xi}(t), \qquad t \geq 0. \tag{5.5}$$

On the other hand, multiplying $\zeta^{ky\cdot\xi}$, $k \in \{1,\dots,n-1\}$ and summing up both sides of (5.4) gives

$$\sum_{y\in X} \zeta^{(k-1)y\cdot\xi}\phi_{y,\xi}(t+1) = -\sum_{y\in X}\zeta^{ky\cdot\xi}\phi_{y,\xi}(t) + 2\rho_{|\xi|}\sum_{y\in X}\phi_{y,\xi}(t), \qquad t \geq 0, \tag{5.6}$$

where we used (4.9). Since $\zeta^{ny\cdot\xi} = 1$, recursive use of (5.6) gives

$$\sum_{y\in X}\phi_{y,\xi}(t) = -\sum_{y\in X}\zeta^{y\cdot\xi}\phi_{y,\xi}(t-1) + 2\rho_{|\xi|}\sum_{y\in X}\phi_{y,\xi}(t-1)$$

$$
\begin{aligned}
&= \sum_{y\in X} \zeta^{2y\cdot\xi}\phi_{y,\xi}(t-2) - 2\rho_{|\xi|}\sum_{y\in X}\phi_{y,\xi}(t-2) + 2\rho_{|\xi|}\sum_{y\in X}\phi_{y,\xi}(t-1) \\
&= (-1)^{n-1}\sum_{y\in X}\zeta^{(n-1)y\cdot\xi}\phi_{y,\xi}(t-n+1) + 2\rho_{|\xi|}\sum_{j=1}^{n-1}(-1)^{j-1}\sum_{y\in X}\phi_{y,\xi}(t-j) \\
&= (-1)^{n-1}\sum_{y\in X}\phi_{y,\xi}(t-n) + 2\rho_{|\xi|}\sum_{j=1}^{n-1}(-1)^{j-1}\sum_{y\in X}\phi_{y,\xi}(t-j), \qquad t\geq n,
\end{aligned}
$$

where (5.5) is used in the last equality. The recurrence relation for

$$
a_{|\xi|}(t) := \sum_{y\in X}\phi_{y,\xi}(t)
$$

is then

$$
a_{|\xi|}(t) = 2\rho_{|\xi|}\sum_{j=1}^{n-1}(-1)^{j-1}a_{|\xi|}(t-j) + (-1)^{n-1}a_{|\xi|}(t-n), \qquad t\geq n \tag{5.7}
$$

with the initial condition

$$
a_{|\xi|}(t) = \frac{1}{\sqrt{n^d}}\big(2\rho_{|\xi|}-1\big)^{t-1}\rho_{|\xi|}, \qquad n>t\geq 1, \qquad a_{|\xi|}(0) = \frac{1}{\sqrt{n^d}}. \tag{5.8}
$$

The characteristic polynomial of the recurrence relation (5.7) is (4.2). The zeros of the characteristic polynomials are denoted by $\mu^{(i)}_{|\xi|}$, $i\in\{1,\dots,n\}$, where $\big|\mu^{(i)}_{|\xi|}\big| = 1$, $i\in\{1,\dots,n\}$ by Lemma 4.1. Moreover, by Proposition 4.2, they are not the negative of the roots of unity $-\zeta^k$, $k\in\mathbb{Z}$. The solution of (5.7) is expressed as

$$
a_{|\xi|}(t) = \frac{1}{\sqrt{n^d}}\sum_{i=1}^{n}c^{(i)}_{|\xi|}\big(\mu^{(i)}_{|\xi|}\big)^t, \qquad t\geq 0 \tag{5.9}
$$

for some constants $c^{(1)}_{|\xi|},\dots,c^{(n)}_{|\xi|}$, $\sum_{i=1}^{n}c^{(i)}_{|\xi|} = 1$. Finding these constants is equivalent to finding the interpolating polynomial satisfying (5.8) at $t=0,1,\dots,n-1$. Namely, we have the matrix equation for $c^{(1)},\dots,c^{(n)}$:

$$
\begin{pmatrix}
1 & 1 & \cdots & 1 \\
\mu^{(1)} & \mu^{(2)} & \cdots & \mu^{(n)} \\
\big(\mu^{(1)}\big)^2 & \big(\mu^{(2)}\big)^2 & \cdots & \big(\mu^{(n)}\big)^2 \\
\vdots & \vdots & \vdots & \vdots \\
\big(\mu^{(1)}\big)^{n-1} & \big(\mu^{(2)}\big)^{n-1} & \cdots & \big(\mu^{(n)}\big)^{n-1}
\end{pmatrix}
\begin{pmatrix} c^{(1)} \\ c^{(2)} \\ c^{(3)} \\ \vdots \\ c^{(n)} \end{pmatrix}
=
\begin{pmatrix} 1 \\ \rho \\ (2\rho-1)\rho \\ \vdots \\ (2\rho-1)^{n-2}\rho \end{pmatrix},
$$

where the subfix $|\xi|$ is omitted for simplicity. The inverse of the Vandermonde matrix in the left-hand side has components

$$
\big[\mu^{j-1}\big]\frac{p(\mu)}{\big(\mu-\mu^{(i)}\big)p'\big(\mu^{(i)}\big)}, \qquad i,j\in\{1,2,\dots,n\},
$$

where $\big[\mu^{j-1}\big]f(\mu)$ represents the coefficient of μ^{j-1} of the polynomial $f(\mu)$, $p(\mu)$ is the polynomial (4.2), and $p'(\mu)$ is its derivative. The solution is (5.1). Substituting (5.9) into (5.4) yields

$$
\phi_{y,\xi}(t) = \frac{1}{\sqrt{n^d}}\frac{w_{|y|}}{\kappa_{|y|}}\left(\big(-\zeta^{-y\cdot\xi}\big)^t - 2\sum_{i=1}^{n}c^{(i)}_{|\xi|}\big(\mu^{(i)}_{|\xi|}\big)^t\sum_{j=1}^{t}\big(-\zeta^{y\cdot\xi}\mu^{(i)}_{|\xi|}\big)^{-j}\right)
$$

$$= \frac{1}{\sqrt{n^d}} \frac{w_{|y|}}{\kappa_{|y|}} \left(\left(-\zeta^{-y\cdot\xi}\right)^t + 2\sum_{i=1}^{n} c^{(i)}_{|\xi|} \frac{\left(\mu^{(i)}_{|\xi|}\right)^t - \left(-\zeta^{-y\cdot\xi}\right)^t}{1+\zeta^{y\cdot\xi}\mu^{(i)}_{|\xi|}} \right)$$

$$= \frac{1}{\sqrt{n^d}} \frac{w_{|y|}}{\kappa_{|y|}} \left[\left(-\zeta^{-y\cdot\xi}\right)^t \left(1 - \sum_{i=1}^{n} \frac{2c^{(i)}_{|\xi|}}{1+\zeta^{y\cdot\xi}\mu^{(i)}_{|\xi|}}\right) + \sum_{i=1}^{n} \frac{2c^{(i)}_{|\xi|}\left(\mu^{(i)}_{|\xi|}\right)^t}{1+\zeta^{y\cdot\xi}\mu^{(i)}_{|\xi|}} \right].$$

In the second equality, we used the fact that $\mu^{(i)}_{|\xi|} \neq -\zeta^k$, $k\in\mathbb{Z}$. The assertion $\tilde{\psi}_{y,0}(t) = \tilde{\psi}_{y,0}(0)$ immediately follows by (5.4) and (5.5). ■

Proof of Theorem 5.1. Since

$$\sum_{l=0}^{n-1} \zeta^{l(a+b)} = n\delta_{a\oplus b,0}, \qquad a,b\in\mathbb{Z},$$

we recast (5.3) into

$$\tilde{\psi}_{y,\xi}(t) = \sqrt{\frac{w_{|y|}}{n^d\kappa_{|y|}}} \sum_{k=0}^{n-1}\sum_{l=0}^{n-1} \frac{\zeta^{l(k-y\cdot\xi)}}{n} \left[\left(-\zeta^{-k}\right)^t \left(1 - \sum_{i=1}^{n} \frac{2c^{(i)}_{|\xi|}}{1+\zeta^{k}\mu^{(i)}_{|\xi|}}\right) + \sum_{i=1}^{n} \frac{2c^{(i)}_{|\xi|}\left(\mu^{(i)}_{|\xi|}\right)^t}{1+\zeta^{k}\mu^{(i)}_{|\xi|}} \right].$$

The inside of the square brackets depends on ξ through $|\xi| = \partial(0,\xi)$, (4.4) yields

$$\psi_{y,x}(t) = \frac{1}{n^d}\sqrt{\frac{w_{|y|}}{\kappa_{|y|}}} \sum_{k=0}^{n-1}\sum_{l=0}^{n-1} \frac{\zeta^{lk}}{n} \Bigg\{ 1 + \sum_{\xi\in X\setminus\{0\}} \zeta^{-(x\oplus ly)\cdot\xi}$$
$$\times \left[\left(-\zeta^{-k}\right)^t \left(1 - \sum_{i=1}^{n} \frac{2c^{(i)}_{|\xi|}}{1+\zeta^{k}\mu^{(i)}_{|\xi|}}\right) + \sum_{i=1}^{n} \frac{2c^{(i)}_{|\xi|}\left(\mu^{(i)}_{|\xi|}\right)^t}{1+\zeta^{k}\mu^{(i)}_{|\xi|}} \right] \Bigg\}$$
$$= \frac{1}{n^d}\sqrt{\frac{w_{|y|}}{\kappa_{|y|}}} \sum_{l=0}^{n-1}\sum_{k=0}^{n-1} \frac{\zeta^{lk}}{n} \Bigg\{ 1 + \sum_{j=1}^{d} K_j(|x\oplus ly|)$$
$$\times \left[\left(-\zeta^{-k}\right)^t \left(1 - \sum_{i=1}^{n} \frac{2c^{(i)}_{j}}{1+\zeta^{k}\mu^{(i)}_{j}}\right) + \sum_{i=1}^{n} \frac{2c^{(i)}_{j}\left(\mu^{(i)}_{j}\right)^t}{1+\zeta^{k}\mu^{(i)}_{j}} \right] \Bigg\}. \quad ■$$

Proof of Corollary 5.2. The contribution from $\rho_0 = 1$ gives unity in the curly brackets, as the last assertion of Proposition 5.3. We begin with the cases with $|\rho_{|\xi|}| < 1$. The recurrence relation (5.7) is

$$a_{|\xi|}(t) - 2\rho_{|\xi|}a_{|\xi|}(t-1) + a_{|\xi|}(t-2) = 0, \qquad t\geq 2$$
$$\text{with } a_{|\xi|}(1) = \frac{\rho_{|\xi|}}{\sqrt{2^d}},\ a_{|\xi|}(0) = \frac{1}{\sqrt{2^d}}.$$

The two zeros of the characteristic polynomial $x^2 - 2\rho_{|\xi|}x + 1$, denoted by $\mu^{+}_{|\xi|}$ and $\mu^{-}_{|\xi|}$, are distinct. We have

$$a_{|\xi|}(t) = \frac{\left(\mu^{+}_{|\xi|}\right)^t + \left(\mu^{-}_{|\xi|}\right)^t}{2\sqrt{2^d}}, \qquad t\geq 0. \tag{5.10}$$

Substituting (5.10) into (5.3) gives

$$\tilde{\psi}_{y,\xi}(t) = \left\{ \frac{\left(\mu^{+}_{|\xi|}\right)^t}{1+(-1)^{y\cdot\xi}\mu^{+}_{|\xi|}} + \frac{\left(\mu^{-}_{|\xi|}\right)^t}{1+(-1)^{y\cdot\xi}\mu^{-}_{|\xi|}} \right\} \tilde{\psi}_{y,\xi}(0).$$

It is convenient to work out for each cases of $z \cdot \xi$ is even or odd:

$$\tilde{\psi}_{y,\xi}(t) = \left\{ \frac{1+(-1)^{y\cdot\xi}}{2} \left[\frac{\left(\mu^+_{|\xi|}\right)^t}{1+\mu^+_{|\xi|}} + \frac{\left(\mu^-_{|\xi|}\right)^t}{1+\mu^-_{|\xi|}} \right] + \frac{1-(-1)^{z\cdot\xi}}{2} \left[\frac{\left(\mu^+_{|\xi|}\right)^t}{1-\mu^+_{|\xi|}} + \frac{\left(\mu^-_{|\xi|}\right)^t}{1-\mu^-_{|\xi|}} \right] \right\} \tilde{\psi}_{y,\xi}(0).$$

This contributes to the inverse Fourier transform as

$$\begin{aligned} &\frac{1}{2^{d+1}} \sqrt{\frac{w_{|y|}}{\kappa_{|y|}}} \sum_{\xi\in\Xi} \left\{ \left[\frac{\left(\mu^+_{|\xi|}\right)^t}{1-\rho_{|\xi|}\mu^+_{|\xi|}} + \frac{\left(\mu^-_{|\xi|}\right)^t}{1-\rho_{|\xi|}\mu^-_{|\xi|}} \right] (-1)^{-x\cdot\xi} \right. \\ &\qquad \left. - \left[\frac{\left(\mu^+_{|\xi|}\right)^{t+1}}{1-\rho_{|\xi|}\mu^+_{|\xi|}} + \frac{\left(\mu^-_{|\xi|}\right)^{t+1}}{1-\rho_{|\xi|}\mu^-_{|\xi|}} \right] (-1)^{-(x\oplus y)\cdot\xi} \right\} \\ &= \frac{1}{2^{d+1}} \sqrt{\frac{w_{|y|}}{\kappa_{|y|}}} \sum_{j=0}^{d} \left\{ \left[\frac{\left(\mu^+_j\right)^t}{1-\rho_j\mu^+_j} + \frac{\left(\mu^-_j\right)^t}{1-\rho_j\mu^-_j} \right] K_j(|x|) \right. \\ &\qquad \left. - \left[\frac{\left(\mu^+_j\right)^{t+1}}{1-\rho_j\mu^+_j} + \frac{\left(\mu^-_j\right)^{t+1}}{1-\rho_j\mu^-_j} \right] K_j(|x\oplus y|) \right\}, \end{aligned}$$

where the last equality follows by Lemma 4.6. For the cases with $\rho_{|\xi|} = \pm 1$, we have

$$\tilde{\psi}_{y,\xi}(t) = \tilde{\psi}_{y,\xi}(0) \begin{cases} 1, & \rho_{|\xi|} = 1, \\ (1-2t)(-1)^t, & \rho_{|\xi|} = -1, \end{cases}$$

for even $y \cdot \xi$ and

$$\tilde{\psi}_{y,\xi}(t) = \tilde{\psi}_{y,\xi}(t) \begin{cases} 1-2t, & \rho_{|\xi|} = 1, \\ (-1)^t, & \rho_{|\xi|} = -1. \end{cases}$$

for odd $y \cdot \xi$. These expressions provide the two last lines of (5.2). Summing up all the contributions, we establish the assertion. ■

6 Limit distributions

Since the probability function $P_t(x)$, $x \in X$ does not converge as $t \to \infty$, Aharonov et al. [1] defined the limit distribution of a quantum walk as the average over infinitely long time

$$\bar{P}(x) = \lim_{T\to\infty} \frac{1}{T} \sum_{t=0}^{T-1} P_t(x) = \lim_{T\to\infty} \frac{1}{T} \sum_{t=0}^{T-1} \sum_{y\in X} |\psi_{y,x}(t)|^2.$$

Intuitively, this quantity captures the proportion of time which the quantum walker spends in state x. In the following calculations, we use

$$\lim_{T\to\infty} \frac{1}{T} \sum_{t=0}^{T-1} \mathrm{e}^{\sqrt{-1}zt} = \delta_{z,0}, \qquad z \in \mathbb{C}.$$

6.1 Hamming graphs $H(d,2)$ (hypercube)

For Hamming graphs $H(d,2)$, we have seen that (5.2) gives an explicit expression of a spectral representation of the wave vector of the quantum walks. Suppose the eigenvalues of the random walk satisfy $|\rho_j| < 1$, $j \in \{1,\dots,d\}$ are distinct, and the eigenvalues of the evolution operator μ_j^+ and μ_j^-, $j \in \{1,\dots,d\}$ are distinct. The mixture of i.i.d. updates for each coordinate (Example 2.5) for generic distribution of α is an example satisfying this assumption. Then, the limit distribution is

$$\begin{aligned}\bar{P}(x) &= \frac{1}{4^d} + \frac{1}{2\cdot 4^d}\sum_{y\in X}\frac{w_{|y|}}{\kappa_{|y|}}\left\{\sum_{j=1}^d\left[\frac{\{K_j(|x|)\}^2}{1-\rho_j^2} + \frac{\{K_j(|x\oplus y|)\}^2}{1-\rho_j^2}\right.\right.\\ &\qquad\left.\left. - \frac{2\rho_j}{1-\rho_j^2}K_j(|x|)K_j(|x\oplus y|)\right]\right\}\\ &= \frac{1}{4^d} + \frac{1}{2\cdot 4^d}\sum_{j=1}^d\{K_j(|x|)\}^2 + \frac{1}{2\cdot 4^d}\sum_{y\in X}\frac{w_{|y|}}{\kappa_{|y|}}\sum_{j=1}^d\frac{\{\rho_jK_j(|x|)-K_j(|x\oplus y|)\}^2}{1-\rho_j^2}\\ &= \frac{\binom{2(d-|x|)}{d-|x|}\binom{2|x|}{|x|}}{2\cdot 4^d\binom{d}{|x|}} + \frac{1}{2\cdot 4^d}\left\{1+\sum_{y\in X}\frac{w_{|y|}}{\kappa_{|y|}}\sum_{j=1}^d\frac{\{\rho_jK_j(|x|)-K_j(|x\oplus y|)\}^2}{1-\rho_j^2}\right\},\end{aligned} \tag{6.1}$$

where we used [9, Theorem 3.1.3]

$$\sum_{j=0}^d\{K_j(|x|)\}^2 = \frac{\binom{2(d-|x|)}{d-|x|}\binom{2|x|}{|x|}}{\binom{d}{|x|}}. \tag{6.2}$$

The expression (6.1) has an interpretation: the limit distribution is the half-and-half mixture of the discrete arcsine law and another probability distribution, because

$$\frac{1}{4^d}\binom{2(d-|x|)}{d-|x|}\binom{2|x|}{|x|}, \qquad |x| \in \{0,1,\dots,d\}$$

is the probability mass function of the discrete arcsine law. The limit distribution (6.1) is has a symmetry,

$$\bar{P}(x) = \bar{P}(1-x), \tag{6.3}$$

because if $n=2$ the identity $K_j(|1-x|) = K_j(d-|x|) = (-1)^j(|x|)$ follows by (2.2).

Example 6.1 (the simple quantum walk)**.** The simple random walk was introduced in Example 2.2. All the eigenvalues of the random walk are distinct and $\rho_d = -1$. For the wave vector of the quantum walk, the last line of (5.2) yields

$$\begin{aligned}&\frac{1}{2^d}\sqrt{\frac{1}{d}}(-1)^t[(1-t)K_d(|x|) - tK_d(|x\oplus y|)]\\ &\quad= \frac{1}{2^d}\sqrt{\frac{1}{d}}(-1)^t\left[(1-t)(-1)^{|x|} - t(-1)^{|x\oplus y|}\right] = \frac{1}{2^d}(-1)^{t+|x|},\end{aligned}$$

since $|y|=1$. The limit distribution is

$$\bar{P}(x) = \frac{\binom{2(d-|x|)}{d-|x|}\binom{2|x|}{|x|}}{2\cdot 4^d\binom{d}{|x|}} + \frac{1}{4^d} + \frac{1}{2d\cdot 4^d}\sum_{j=1}^{d-1}\frac{\sum_{y:\,|y|=1}\{\rho_jK_j(|x|)-K_j(|x\oplus y|)\}^2}{1-\rho_j^2}.$$

This coincides with equation 13 in Ho et al. [10] by the following identity. This limit distribution has the symmetry (6.3).

Proposition 6.2. *For* $j \in \{1, \ldots, d-1\}$ *and* $\rho_j = 1 - 2j/d$,

$$\sum_{z\colon |z|=1} \{\rho_j K_j(|x|) - K_j(|x \oplus z|)\}^2 = \left(1 - \frac{|x|}{d}\right) |x| \{K_j(|x|-1) - K_j(|x|+1)\}^2, \tag{6.4}$$

where $x \in X$.

Proof. If $|x| = 0$ or d, the equality holds because $\rho_j K_j(0) = K_j(1)$ and $\rho_j K_j(d) = K_j(d-1)$, respectively. Otherwise, expanding the left-hand side of (6.4) yields

$$\begin{aligned} &d\{\rho_j K_j(|x|)\}^2 - 2\rho_j K_j(|x|)\{(d-|x|)K_j(|x|+1) + |x|K_j(|x|-1)\} \\ &\qquad + (d-|x|)\{K_j(|x|+1)\}^2 + |x|\{K_j(|x|-1)\}^2. \end{aligned}$$

We recast this into the right-hand side of (6.4) by expressing $K_j(|x|)$ with $K_j(|x|-1)$ and $K_j(|x|+1)$ by using the three-term recurrence relation of the Krawtchouk polynomials [12, equation (1.10.3)]:

$$\frac{i}{d} K_j(i-1) + \left(1 - \frac{i}{d}\right) K_j(i+1) = \left(1 - \frac{2j}{d}\right) K_j(i), \qquad i \in \{1, \ldots, d-1\}. \qquad \blacksquare$$

Example 6.3 (the independent quantum walk)**.** The independent random walk was introduced in Example 2.3. The eigenvalues of this random walk degenerate. For the quantum walk, the wave vector is

$$\begin{aligned} \psi_{y,x}(t) = \frac{1}{2^{3d/2}} \Bigg\{ 1 + \frac{1}{2} \left[\left(\sqrt{-1}\right)^t + \left(-\sqrt{-1}\right)^t \right] \left(2^d \delta_{|x|,0} - 1\right) \\ - \frac{1}{2} \left[\left(\sqrt{-1}\right)^{t+1} + \left(-\sqrt{-1}\right)^{t+1} \right] \left(2^d \delta_{|x \oplus y|,0} - 1\right) \Bigg\}. \end{aligned}$$

The limit distribution is

$$\bar{P}(x) = \left(\frac{1}{2} - \frac{1}{2^d}\right) \delta_{x,0} + \frac{1}{2 \cdot 2^d} + \frac{1}{4^d}.$$

As $d \to \infty$, this is the half-and-half mixture of the atom at the origin and the uniform distribution. The limit distribution does not have the symmetry (6.3).

Example 6.4 (the non-local quantum walk)**.** The non-local random walk was introduced in Example 2.4. To make the expressions explicit, let the cardinality $m = 2$ and assume $d \geq 3$ is odd. Then,

$$\rho_i = \frac{K_2(i)}{\kappa_2} = 1 - \frac{4i}{d-1} + \frac{4i^2}{d(d-1)} > -\frac{1}{d-1}, \qquad i \in \{0, \ldots, d\},$$

where $\rho_i = \rho_{d-i}$, $i \in \{0, \ldots, d\}$. For the wave vector of the quantum walk, the second last line of (6.1) yields

$$\begin{aligned} &\frac{1}{2^d} \sqrt{\frac{2}{d(d-1)}} [(1-t)K_d(|x|) - tK_d(|x \oplus y|)] \\ &\qquad = \frac{1}{2^d} \sqrt{\frac{2}{d(d-1)}} \left[(1-t)(-1)^{|x|} - t(-1)^{|x \oplus y|}\right] = \frac{1}{2^d} \sqrt{\frac{2}{d(d-1)}} (-1)^{|x|}, \end{aligned}$$

since $|y|=2$. The limit distribution is

$$\bar{P}(x)=\frac{\binom{2(d-|x|)}{d-|x|}\binom{2|x|}{|x|}}{2\cdot 4^d\binom{d}{|x|}}+\frac{1}{4^d}$$
$$+\frac{1}{4^d}\frac{2}{d(d-1)}\sum_{j=1}^{(d-1)/2}\frac{\sum_{y:\,|y|=2}\{\rho_j K_j(|x|)-K_j(|x\oplus y|)\}^2}{1-\rho_j^2},$$

which has the symmetry (6.3).

Example 6.5 (the mixture of i.i.d. updates for each coordinate)**.** The limit distribution is the mixture of (6.1) with the distribution of parameter $\alpha\in(0,1)$. If it has the single atom at $r\in(0,1)\setminus\{1/2\}$, we have

$$\bar{P}(x)=\frac{\binom{2(d-|x|)}{d-|x|}\binom{2|x|}{|x|}}{2\cdot 4^d\binom{d}{|x|}}+\frac{1}{2\cdot 4^d}$$
$$+\frac{1}{2\cdot 4^d}\sum_{y\in X}r^{|y|}(1-r)^{d-|y|}\sum_{j=1}^{d}\frac{\{(1-2r)^j K_j(|x|)-K_j(|x\oplus y|)\}^2}{1-(1-2r)^j}, \tag{6.5}$$

which has the symmetry (6.3). If $r=1/2$, this model reduces to Example 6.3, where the eigenvalues of the random walk degenerate, while (6.5) reduces to the half-and-half mixture of the discrete arcsine law and the uniform distribution, where we used

$$\sum_{y\in X}\sum_{j=0}^{d}\{K_j(|y|)\}^2=\sum_{i=0}^{d}\binom{2(d-i)}{d-i}\binom{2i}{i}=4^d.$$

Here, the first equality follows by (6.2), and the second equality can be obtained by noting that

$$\sum_{i=0}^{\infty}\binom{2i}{i}s^i=\frac{1}{\sqrt{1-4s}}.$$

Figure 1 displays the limit distributions of quantum walks for $d=10$. Independent quantum walk (Example 6.3) and i.i.d. updates with a single atom at $r=0.1$, $r=0.49$, and $r=0.9$ are shown. When r is close to 0 or 1, large probability masses are concentrated around 0 and $(1,\dots,1)$. These are similar to the simple quantum walks (Example 6.1) in that they are concave in the center (see [14, Figure 2]). If $r=0.49$, the limit distribution is close to the half-and-half mixture of the discrete arcsine law and the uniform distributions, but if $r=1/2$ (the independent quantum walk), the symmetry (6.3) breaks down and the component other than the uniform distribution is piled up at the origin. This drastic change of the behaviour at $r=1/2$ is reminiscent of the fact that the random walk mixes in exactly one step at $r=1/2$.

6.2 Hamming graphs $H(d,n)$ for prime $n\geq 3$

We prepare the following identities.

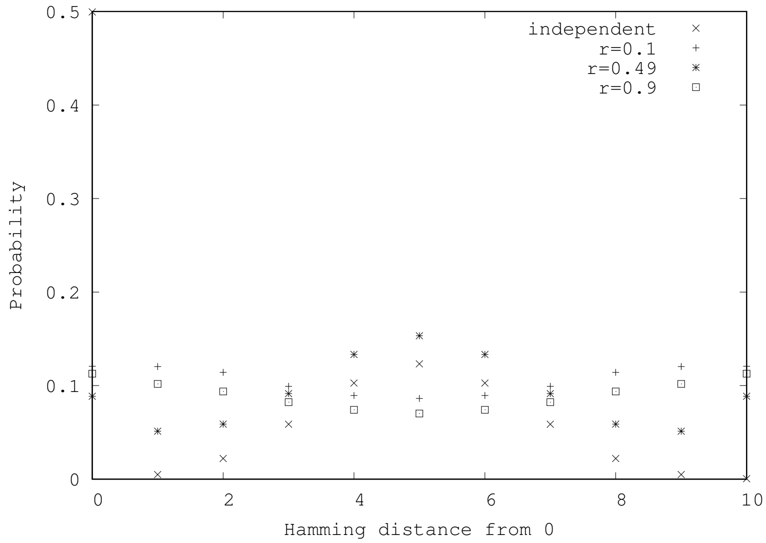

Figure 1. The limit distributions of some quantum walks.

Proposition 6.6. *For odd $n \geq 3$, we have*

$$\sum_{k=0}^{n-1} \frac{1}{1+\zeta^k} = \frac{n}{2}, \tag{6.6}$$

$$\sum_{k=0}^{n-1} \frac{\zeta^{lk}}{1+\zeta^k} = \frac{n}{2}(-1)^{l-1}, \qquad l \in \{1, \dots, n-1\}, \tag{6.7}$$

$$\sum_{k=0}^{n-1} \frac{1}{\left(1+\zeta^k\right)\left(1+\bar{\zeta}^k\right)} = \frac{n^2}{4}, \tag{6.8}$$

where $\zeta = \mathrm{e}^{2\pi\sqrt{-1}/n}$.

Proof. Note that

$$\frac{2}{1+\zeta^k} = \frac{1-\left(-\zeta^k\right)^n}{1-\left(-\zeta^k\right)} = \sum_{i=0}^{n-1}\left(-\zeta^k\right)^i.$$

For (6.6), we have

$$\frac{1}{2}\sum_{k=0}^{n-1}\sum_{i=0}^{n-1}(-1)^i\zeta^{ki} = \frac{n}{2} + \frac{1}{2}\sum_{i=1}^{n-1}(-1)^i\sum_{k=0}^{n-1}\zeta^{ki} = \frac{n}{2} + \frac{1}{2}\sum_{i=1}^{n-1}(-1)^i\frac{1-\zeta^{in}}{1-\zeta^i} = \frac{n}{2}.$$

For (6.7), we have

$$\begin{aligned}\frac{1}{2}\sum_{k=0}^{n-1}\sum_{i=0}^{n-1}(-1)^i\zeta^{k(i+l)} &= \frac{n}{2}(-1)^{n-l} + \frac{1}{2}\sum_{i\in\{0,\dots,n-1\}\setminus\{n-l\}}(-1)^i\sum_{k=0}^{n-1}\zeta^{k(i+l)} \\ &= \frac{n}{2}(-1)^{n-l} + \frac{1}{2}\sum_{i\in\{0,\dots,n-1\}\setminus\{n-l\}}(-1)^i\frac{1-\zeta^{(i+l)n}}{1-\zeta^{i+l}} = \frac{n}{2}(-1)^{l+1}.\end{aligned}$$

For (6.8), we have

$$\sum_{k=0}^{n-1}\frac{1}{\left(1+\zeta^k\right)\left(1+\bar{\zeta}^k\right)} = \frac{1}{4}\sum_{k=0}^{n-1}\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}\left(-\zeta^k\right)^i\left(-\zeta^{-k}\right)^j = \frac{1}{4}\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}\left(-\zeta^k\right)^{i-j}$$

$$= \frac{1}{4}\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}(-1)^{i-j}\sum_{k=0}^{n-1}\left(\zeta^{i-j}\right)^k$$
$$= \frac{1}{4}\sum_{i=0}^{n-1} n + \frac{1}{4}\sum_{i=0}^{n-1}\sum_{j\in\{0,\dots,n-1\}\setminus\{i\}}(-1)^{i-j}\frac{1-\zeta^{(i-j)n}}{1-\zeta^{i-j}} = \frac{n^2}{4}. \qquad \blacksquare$$

With using these identities, we obtain the following example.

Example 6.7 (the independent quantum walk)**.** The wave vector is

$$\psi_{y,x}(t) = \frac{1}{n^{3d/2}}\sum_{l=0}^{n-1}\sum_{k=0}^{n-1}\frac{\zeta^{lk}}{n}\left[1 + \frac{2}{n}\left(n^d\delta_{|x\oplus ly|,0} - 1\right)\sum_{i=0}^{n-1}\frac{\zeta^{it}}{1+\zeta^{ik}}\right].$$

The limit distribution is

$$\bar{P}(x) = \left(1 - \frac{1}{n}\right)\frac{1}{n^d} + \frac{2(n-1)}{n^{2d+1}} + \left(\frac{1}{n} - \frac{2(n-1)}{n^{d+1}}\right)\delta_{x,0}.$$

As $d \to \infty$, this is the $(1-1/n)$-and-$1/n$ mixture of the uniform distribution and the atom at the origin.

The spectral representations for $n \geq 3$ becomes much more involved than those for $n = 2$. For the simple random walk of $n = 3$, the eigenvalues are

$$\rho_0 = 1, \qquad \rho_d = -1/2, \qquad \text{and} \qquad \rho_j = 1 - \frac{3j}{2d}, \qquad j \in \{1, 2, \dots, d-1\},$$

where $\rho_j \in (-1/2, 1)$, $j \in \{1, 2, \dots, d-1\}$. The corresponding eigenvalues of the evolution operator of the quantum walk are

$$\begin{array}{ll} 1,\ -\zeta,\ -\zeta^2 & \text{for } \rho_0 = 1, \\ 1,\ -1 & \text{for } \rho_d = -1/2, \\ 1,\ \mathrm{e}^{\pm\sqrt{-1}\theta_j} & \text{for } \rho_j,\ j \in \{1, 2, \dots, d-1\}, \end{array}$$

where

$$\cos\theta_j = \rho_j - \frac{1}{2} = \frac{d-3j}{2d}.$$

For $j \in \{1, 2, \dots, d-1\}$,

$$c_j^{(1)} = \frac{d}{d+3j}, \qquad c_j^{(2)} = c_j^{(3)} = \frac{3j}{2(d+3j)}.$$

Since $\rho_d = -1/2$ violates the assumption of Theorem 5.1, we consider the contribution separately. The same argument to obtain Proposition 5.3 yields

$$\tilde{\psi}_{y,\xi}(t) = \frac{1}{\sqrt{3^d \cdot 2d}}\sum_{k=1}^{2}\sum_{l=0}^{2}\frac{\zeta^{l(k-y\cdot\xi)}}{6}\left[\frac{1}{1+\zeta^k} - \frac{3(-1)^t}{1-\zeta^k} + \frac{2\left(2+2\zeta^k-\zeta^{2k}\right)}{1-\zeta^{2k}}\left(-\zeta^{3-k}\right)^t\right]$$

for $|\xi| = d$, where we used the fact that $y \cdot \xi \neq 0$ if $|\xi| = d$ and $|y| = 1$. Then, the wave vector is

$$\psi_{y,x}(t) = \frac{1}{3^d\sqrt{2d}}\sum_{k=0}^{2}\sum_{l=0}^{2}\frac{\zeta^{lk}}{3}$$

$$\times\left[1+\sum_{j=1}^{d-1}K_j(|x\oplus ly|)\left(\frac{2c_j^{(1)}}{1+\zeta^k}+\frac{2c_j^{(2)}\mathrm{e}^{\sqrt{-1}\theta_j t}}{1+\zeta^k\mathrm{e}^{\sqrt{-1}\theta_j}}+\frac{2c_j^{(2)}\mathrm{e}^{-\sqrt{-1}\theta_j t}}{1+\zeta^k\mathrm{e}^{-\sqrt{-1}\theta_j}}\right)\right]$$
$$+\frac{1}{3^d\sqrt{2d}}\sum_{k=1}^{2}\sum_{l=0}^{2}\frac{\zeta^{lk}}{6}K_d(|x\oplus ly|)\left[\frac{1}{1+\zeta^k}-\frac{3(-1)^t}{1-\zeta^k}+\frac{2\big(2+2\zeta^k-\zeta^{2k}\big)}{1-\zeta^{2k}}\big(-\zeta^{3-k}\big)^t\right].$$

We have

$$\psi_{y,x}(t)=\frac{1}{3^d\sqrt{2d}}\Bigg\{1+\sum_{j=1}^{d-1}c_j^{(1)}[K_j(|x|)+K_j(|x\oplus y|)-K_j(|x\oplus 2y|)]$$
$$+\frac{1}{6}[K_d(|x|)+K_d(|x\oplus y|)-2K_d(|x\oplus 2y|)]-\frac{1}{2}[K_d(|x|)-K_d(|x\oplus y|](-1)^t$$
$$+\big[K_d(|x|)+\zeta K_d(|x\oplus y|)+\zeta^2K_d(|x\oplus 2y|)\big]\frac{\big(-\zeta^2\big)^t}{1-\zeta}$$
$$-\big[\zeta K_d(|x|)+K_d(|x\oplus y|)+\zeta^2K_d(|x\oplus 2y|)\big]\frac{(-\zeta)^t}{1-\zeta}$$
$$+\sum_{j=1}^{d-1}\big[K_j(|x|)+K_j(|x\oplus y|)\mathrm{e}^{2\sqrt{-1}\theta_j}+K_j(|x\oplus 2y|)\mathrm{e}^{\sqrt{-1}\theta_j}\big]\frac{2c_j^{(2)}\mathrm{e}^{\sqrt{-1}\theta_j t}}{1+\mathrm{e}^{3\sqrt{-1}\theta_j}}$$
$$+\sum_{j=1}^{d-1}\big[K_j(|x|)+K_j(|x\oplus y|)\mathrm{e}^{-2\sqrt{-1}\theta_j}+K_j(|x\oplus 2y|)\mathrm{e}^{-\sqrt{-1}\theta_j}\big]\frac{2c_j^{(2)}\mathrm{e}^{-\sqrt{-1}\theta_j t}}{1+\mathrm{e}^{-3\sqrt{-1}\theta_j}}\Bigg\}.$$

The limit distribution is

$$\bar{P}(x)=\frac{1}{9^d}+\frac{4^{d-|x|}}{9^d}\frac{17d+45|x|}{8d}-\left(\frac{2}{9}\right)^d\left(-\frac{1}{2}\right)^{|x|+1}+\frac{2}{9^d}\sum_{j=1}^{d-1}\frac{K_j(|x|)}{1+3j/d}$$
$$+\frac{1}{2d\cdot 9^d}\sum_{y:\,|y|=1}\left[\sum_{j=1}^{d-1}\frac{K_j(|x|)+K_j(|x\oplus y|)-K_j(|x\oplus 2y|)}{1+3j/d}\right]^2$$
$$+\frac{2^d}{12d\cdot 9^d}\sum_{j=1}^{d-1}\sum_{y:|y|=1}\frac{K_j(|x|)+K_j(|x\oplus y|)-K_j(|x\oplus 2y|)}{1+3j/d}$$
$$\times\left[\left(-\tfrac{1}{2}\right)^{|x|}+\left(-\tfrac{1}{2}\right)^{|x\oplus y|}-2\left(-\tfrac{1}{2}\right)^{|x\oplus 2y|}\right]$$
$$+\frac{1}{3\cdot 9^d}\sum_{j=1}^{d-1}\frac{1}{d-j}\sum_{y:|y|=1}\left|\frac{K_j(|x|)+K_j(|x\oplus y|)\mathrm{e}^{2\sqrt{-1}\theta_j}+K_j(|x\oplus 2y|)\mathrm{e}^{\sqrt{-1}\theta_j}}{1+3j/d}\right|^2,$$

where we used $K_d(j)=2^d(-1/2)^j$, $j\in\{0,1,\dots,d\}$ and Table 1.

Table 1. $|x\oplus y|$ and $|x\oplus 2y|$ for $|y|=1$, $y_i\neq 0$.

		$\lvert x\oplus y\rvert$	$\lvert x\oplus 2y\rvert$
$x_i=0$		$\lvert x\rvert+1$	$\lvert x\rvert+1$
$x_i=1$	$y_i=1$	$\lvert x\rvert$	$\lvert x\rvert-1$
$x_i=1$	$y_i=2$	$\lvert x\rvert-1$	$\lvert x\rvert$
$x_i=2$	$y_i=1$	$\lvert x\rvert-1$	$\lvert x\rvert$
$x_i=2$	$y_i=2$	$\lvert x\rvert$	$\lvert x\rvert-1$

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