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Mixture of Gaussians in the open quantum random walks

Chul Ki Ko[1] · **Hyun Jae Yoo**[2]

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Abstract

We discuss the Gaussian and the mixture of Gaussians in the limit of open quantum random walks. The central limit theorems for the open quantum random walks under certain conditions were proven by Attal et al (Ann Henri Poincaré 16(1):15–43, 2015) on the integer lattices and by Ko et al (Quantum Inf Process 17(7):167, 2018) on the crystal lattices. The purpose of this paper is to investigate the general situation. We see that the Gaussian and the mixture of Gaussians in the limit depend on the structure of the invariant states of the intrinsic quantum Markov semigroup whose generator is given by the Kraus operators which generate the open quantum random walks. Some concrete models are considered for the open quantum random walks on the crystal lattices. Due to the intrinsic structure of the crystal lattices, we can conveniently construct the dynamics as we like. Here, we consider the crystal lattices of $\mathbb{Z}^2$ with intrinsic two points, hexagonal, triangular, and Kagome lattices. We also discuss Fourier analysis on the crystal lattices which gives another method to get the limit theorems.

Keywords Open quantum random walks · Quantum dynamical semigroup · Invariant states · Crystal lattices · Central limit theorem · Mixture of Gaussians

Mathematics Subject Classification 82B41 · 82C41

✉ Hyun Jae Yoo
yoohj@hknu.ac.kr

Chul Ki Ko
kochulki@yonsei.ac.kr

1 University College, Yonsei University, 85 Songdogwahak-ro, Yeonsu-gu, Incheon 21983, Korea

2 School of Computer Engineering and Applied Mathematics, and Institute for Integrated Mathematical Sciences, Hankyong National University, 327 Jungang-ro, Anseong-si, Gyeonggi-do 17579, Korea

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1 Introduction

In this paper, we investigate the limit distributions of the open quantum random walks (OQRWs hereafter) [1–3,8]. The limit distributions of OQRWs have been investigated in several papers. See, for instance, references [1,2,7,9]. The central limit theorem (CLT in short) was firstly shown in [1] for OQRWs on the integer lattices, and then, it was shown for models on the crystal lattices in [8]. In both cases, in order that the CLT holds, a certain condition must be provided. Recall that the OQRWs consist of repeated two dynamics: an intrinsic change of states followed by space movements. Considering solely the intrinsic dynamics, it defines a quantum Markov semigroup (QMS shortly). The condition for the CLT is that the QMS should be irreducible and thereby there exists only one invariant state for the QMS. We refer to Sect. 3 for the details. One naturally then asks what would be the limit distribution of the OQRWs if the irreducibility fails to hold. It is the main motivation of this paper to answer this question.

After demonstrating some known results on the structure of invariant states for QMSs [4–6,11,12], we show that in general we get a mixture of Gaussians for the limit distributions of OQRWs. For the models, we consider the OQRWs on the crystal lattices. One notices that the crystal lattices extend the integer lattices (see Sect. 2.1). Since they have rich intrinsic structure, it is very convenient to set up many interesting models on them. The crystal lattices considered here are the $\mathbb{Z}^2$ with intrinsic two points, hexagonal, triangular, and Kagome lattices. In [8], we mainly dealt with hexagonal lattices to construct OQRWs showing CLT. In this paper, we further consider the triangular and Kagome lattices satisfying the central limit theorems (see "Appendix A"). As for the mixture of Gaussians, we consider some models on $\mathbb{Z}^2$ with intrinsic two points and a model on the hexagonal lattice (Sect. 4.3). We would like to stress that the models considered here serve as good examples for understanding the structure of the invariant states for the QMSs.

The paper is organized as follows: In Sect. 2, we briefly recall the basic preliminaries that was introduced in [8]. Namely, we review the definition of the crystal lattices and the construction of OQRWs on the crystal lattices. In Sect. 3, we recall the central limit theorem for the OQRWs on the crystal lattices. The models of CLT will be demonstrated in "Appendix." In Sect. 4, we deal with the situation where a mixture of Gaussians appears. In Sect. 4.1, we review some known results on the structure of invariant states for QMSs. We apply the theory to the OQRWs and investigate the limit distributions of OQRWs in Sect. 4.2 and give some examples in Sect. 4.3. In Sect. 5, we summarize what we have discussed in the main body of the paper. In "Appendix A," we provide with some models that reveal CLT on the triangular and Kagome lattices. The method of Fourier analysis, which gives an analytic proof of the limit distribution, is given in "Appendix B" proving the same result obtained in the body.

2 Preliminaries

In this section, for the readers' convenience, we briefly review the OQRWs on the crystal lattices established in [8].

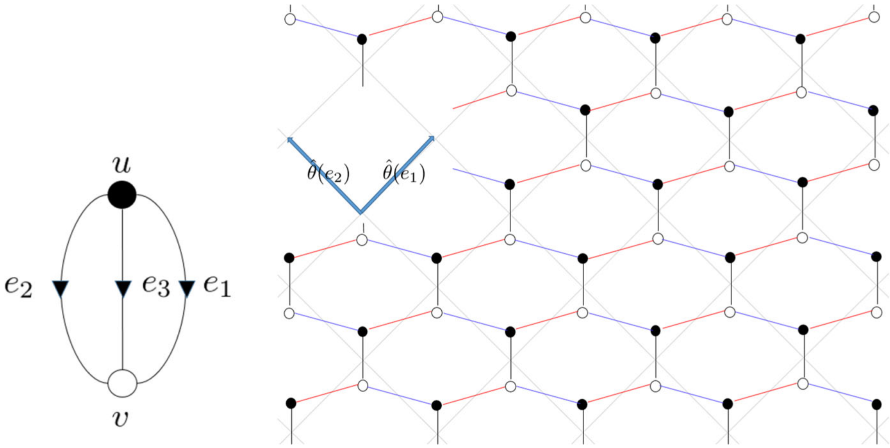

Fig. 1 Hexagonal lattice: underlying graph G_0 for hexagonal lattice (left) and hexagonal lattice (right)

2.1 Crystal lattices

In this subsection, we briefly introduce the crystal lattices summarized in [7]. Let $G_0 = (V_0, E_0)$ be a finite graph possibly having multi-edges and self-loops. We use the notation $A(G_0)$ for the set of symmetric arcs induced by E_0. The homology group of G_0 with integer coefficients is denoted by $H_1(G_0, \mathbb{Z})$. The abstract periodic lattice $\mathbb{L}$ induced by a subgroup $H \subset H_1(G_0, \mathbb{Z})$ is denoted by $H_1(G_0, \mathbb{Z})/H$ [10]. Let $\{C_1, C_2, \ldots, C_{b_1}\}$ be the fundamental cycles of G_0 which constitutes the basis of $H_1(G_0, \mathbb{Z})$, where b_1 is the first Betti number of G_0. The spanning tree induced by $\{C_1, C_2, \ldots, C_{b_1}\}$ is denoted by $\mathbb{T}_0$. We notice that there is a one-to-one correspondence between $\{C_1, C_2, \ldots, C_{b_1}\}$ and $A(\mathbb{T}_0)^c$; we describe $C(e) \in \{C_1, C_2, \ldots, C_{b_1}\}$ as the fundamental cycle corresponding to $e \in A(\mathbb{T}_0)^c$ so that $C(e)$ is the cycle generated by adding e to $\mathbb{T}_0$. Let d be the number of generators of the quotient group $H_1(G_0, \mathbb{Z})/H$. By taking a set of generating vectors $\{\widehat{\theta}(e) : e \in A(\mathbb{T}_0)^c\}$ (we suppose $\widehat{\theta}(\bar{e}) = -\widehat{\theta}(e)$, where $\bar{e}$ means the reversed arc of e), we may consider $\mathbb{L}$ as a subset of $\mathbb{R}^d$ isomorphic to $\mathbb{Z}^d$. In other words, we may think

$$\mathbb{L} = \left\{ \sum n_e \widehat{\theta}(e) : e \in A(\mathbb{T}_0)^c,\ n_e \in \mathbb{Z} \right\}.$$

The covering graph $G = (V, A)$ of G_0, which is called a crystal lattice, is defined as follows. First, we define a map $\phi_0 : V_0 \to \mathbb{R}^d$. The covering graph $G = (V, A)$ is defined as follows:

$$\begin{aligned} V &= \mathbb{L} + \phi_0(V_0) \cong \mathbb{L} \times \phi_0(V_0); \\ A &= \cup_{x \in \mathbb{L}} \{((x, \mathrm{o}(e)), (x, \mathrm{t}(e))) \mid e \in A(\mathbb{T}_0)\} \\ &\quad \cup \left(\cup_{x \in \mathbb{L}} \left\{ \left((x, \mathrm{o}(e)), (x + \widehat{\theta}(e), \mathrm{t}(e))\right) \mid e \in A(\mathbb{T}_0)^c \right\} \right). \end{aligned}$$

Here, $\mathrm{o}(e)$ and $\mathrm{t}(e)$ mean the origin and terminus of e, respectively.

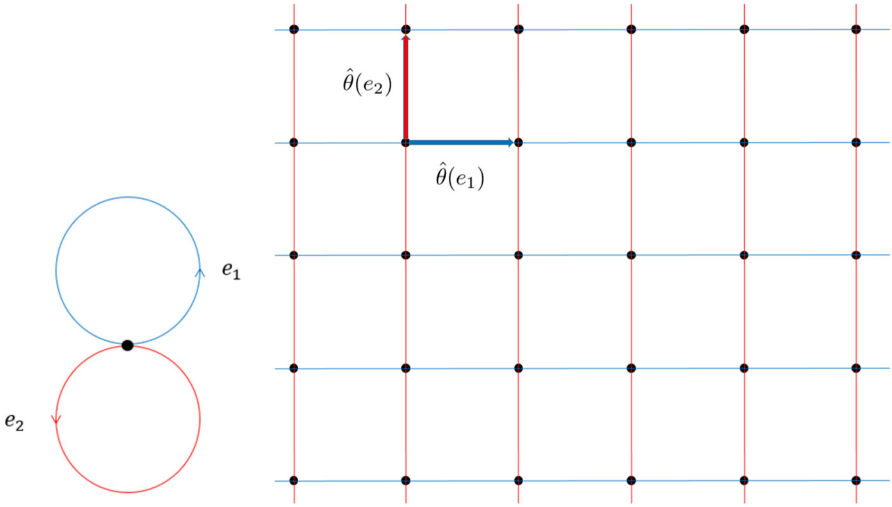

Fig. 2 $\mathbb{Z}^2$ as a crystal lattice

We take $\widehat{\theta}(e) \equiv 0$ for $e \in A(\mathbb{T}_0)$ and choose $e_{i_1}, \ldots, e_{i_d}$ from $A(\mathbb{T}_0)^c$ so that $\widehat{\theta}_1 := \widehat{\theta}(e_{i_1}), \ldots, \widehat{\theta}_d := \widehat{\theta}(e_{i_d})$ span $\mathbb{R}^d$. We further suppose that for all $e \in A(G_0)$, $\widehat{\theta}(e) \in \{\sum_{i=1}^d n_i \widehat{\theta}_i : n_i \in \mathbb{Z},\ i = 1, \cdots, d\}$, and for any two arcs e_i and e_j in $A(\mathbb{T}_0)^c$, $\widehat{\theta}(e_i)$ and $\widehat{\theta}(e_j)$ are linearly independent unless $e_j = \overline{e}_i$. We define a $d \times d$ matrix by

$$\Theta := ([\widehat{\theta}_1, \ldots, \widehat{\theta}_d]^{-1})^T. \tag{2.1}$$

Notice that if $\{\mathbf{e}_i : i = 1, \cdots, d\}$ is the canonical basis for $\mathbb{R}^d$, then we have

$$\mathbf{e}_i = \sum_{j=1}^{d} \Theta_{ij} \widehat{\theta}_j. \tag{2.2}$$

Before ending this subsection, we remark that the integer lattices are the special crystal lattices as can be seen in Fig. 2.

2.2 OQRWs on the crystal lattices

The Hilbert space for the OQRWs on the crystal lattices has the form $\mathfrak{h} \otimes \mathcal{K}$, where $\mathcal{K} := l^2(\mathbb{L})$ with a canonical orthonormal basis $\{|x\rangle : x \in \mathbb{L}\}$, and $\mathfrak{h} := \oplus_{u \in V_0} \mathfrak{h}_u$ with $\mathfrak{h}_u$, $u \in V_0$, being a copy of a finite-dimensional Hilbert space $\mathfrak{h}_0$.

Whenever there is no danger of confusion, we also understand $\mathfrak{h}_u$ as a subspace of $\mathfrak{h}$. For each $e \in A(G_0)$, $e = (u, v)$, we let $B(e)$ be a bounded linear operator on $\mathfrak{h}$ such that $\mathrm{Dom}(B(e)) = \mathfrak{h}_u$ and $\mathrm{Ran}(B(e)) \subset \mathfrak{h}_v$, and it satisfies

$$\sum_{\substack{e\in A(G_0);\\ \mathrm{o}(e)=u}} B^*(e)B(e) = I_{\mathfrak{h}_u} \quad \text{for all } u \in V_0. \tag{2.3}$$

We easily check that

$$\sum_{e\in A(G_0)} B^*(e)B(e) = \sum_{u\in V_0} \sum_{\substack{e\in A(G_0);\\ \mathrm{o}(e)=u}} B^*(e)B(e) = \sum_{u\in V_0} I_{\mathfrak{h}_u} = I_{\mathfrak{h}}. \tag{2.4}$$

The operators $\{B(e) : e \in A(G_0)\}$ will constitute the Kraus representation of our OQRWs on the crystal lattices. For that we define for each $x \in \mathbb{L}$ and $e \in A(G_0)$, a bounded linear operator L_x^e on $\mathfrak{h} \otimes \mathcal{K}$ by

$$L_x^e := B(e) \otimes |x + \widehat{\theta}(e)\rangle\langle x|. \tag{2.5}$$

We can check (see [8, Lemma 2.1])

$$\sum_{x\in\mathbb{L}} \sum_{e\in A(G_0)} \left(L_x^e\right)^* L_x^e = I_{\mathfrak{h}\otimes\mathcal{K}}. \tag{2.6}$$

The OQRW is a completely positive linear operator on the ideal $\mathcal{I}_1(\mathfrak{h}\otimes\mathcal{K})$ of trace class operators on $\mathfrak{h}\otimes\mathcal{K}$ defined by

$$\mathcal{M}(\rho) := \sum_{x\in\mathbb{L}} \sum_{e\in A(G_0)} L_x^e \rho (L_x^e)^*. \tag{2.7}$$

Let us consider a special class of states (density operators) on $\mathfrak{h}\otimes\mathcal{K}$ of the form

$$\rho = \sum_{x\in\mathbb{L}} \left(\oplus_{u\in V_0} \rho_{(x,u)}\right) \otimes |x\rangle\langle x|. \tag{2.8}$$

Here, for each pair $(x, u) \in \mathbb{L} \times V_0$, $\rho_{(x,u)}$ is a positive definite operator on $\mathfrak{h}_u$ and satisfies

$$\sum_{x\in\mathbb{L}} \sum_{u\in V_0} \mathrm{Tr}(\rho_{(x,u)}) = 1.$$

The value $\sum_{u\in V_0} \mathrm{Tr}(\rho_{(x,u)})$ is understood as a probability of finding the particle at site $x \in \mathbb{L}$ when the state is ρ. We check that if the state has the form in (2.8), $\rho = \sum_{x\in\mathbb{L}} \left(\oplus_{u\in V_0} \rho_{(x,u)}\right) \otimes |x\rangle\langle x|$, $\mathcal{M}(\rho)$ has the form

$$\mathcal{M}(\rho) = \sum_{x\in\mathbb{L}} \left(\oplus_{u\in V_0} \rho'_{(x,u)}\right) \otimes |x\rangle\langle x|, \tag{2.9}$$

where

$$\rho'_{(x,u)} = \sum_{\substack{e \in A(G_0); \\ \mathrm{t}(e)=u}} B(e)\rho_{(x-\widehat{\theta}(e),\mathrm{o}(e))} B(e)^*.$$

From now on, we assume that $\mathcal{M}$ is defined on the set of states of the form in (2.8).

As was introduced in [1,2], let $(\rho_n, X_n)_{n\geq 0}$ denote the Markov chain of quantum trajectory procedure. This is obtained by repeatedly applying the completely positive map $\mathcal{M}$ and a measurement of the position on $\mathcal{K}$. More precisely, denoting $\mathcal{E}(\mathfrak{h})$ the space of states on $\mathfrak{h}$, $(\rho_n, X_n)_{n\geq 0}$ is a Markov chain on the state space $\mathcal{E}(\mathfrak{h}) \times \mathbb{L}$ for which the transition rule is defined as follows: From a point $(\rho, x) \in \mathcal{E}(\mathfrak{h}) \times \mathbb{L}$, it jumps to the point

$$\left(\frac{1}{p(e)} B(e)\rho B(e)^*, x + \widehat{\theta}(e) \right) \in \mathcal{E}(\mathfrak{h}) \times \mathbb{L},$$

with probability

$$p(e) = \mathrm{Tr}(B(e)\rho B(e)^*).$$

3 Central limit theorem

In this section, we review the central limit theorem for the OQRWs on the crystal lattices, which was developed in [8]. The same study for the OQRWs on the integer lattices $\mathbb{Z}^d$ was done in [1]. Let us consider the Markov generator

$$\mathcal{L}_*(\rho) := \sum_{e \in A(G_0)} B(e)\rho B(e)^* - \rho, \quad \rho \in \mathcal{I}_1(\mathfrak{h}). \tag{3.1}$$

Here, $\mathcal{I}_1(\mathfrak{h})$ is the space of trace class operators on $\mathfrak{h}$.

We assume the following hypothesis.

(H1) The equation $\mathcal{L}_*(\rho) = 0$ has a unique solution ρ_∞ among the state space $\mathcal{E}(\mathfrak{h})$.

The CLT for the OQRWs on the crystal lattices developed in [8] reads as follows. Let us define

$$m := \sum_{e \in A(G_0)} \mathrm{Tr}\left(B(e)\rho_\infty B(e)^*\right) \widehat{\theta}(e). \tag{3.2}$$

Lemma 3.1 *For any $l \in \mathbb{R}^d$, the equation ($\mathcal{L} := (\mathcal{L}_*)^*$)*

$$-\mathcal{L}(L) = \sum_{e \in A(G_0)} B(e)^* B(e) \left(\widehat{\theta}(e) \cdot l\right) - (m \cdot l)I \tag{3.3}$$

for $L \in \mathcal{B}(\mathfrak{h})$, the space of bounded linear operators on $\mathfrak{h}$, admits a solution. The difference between any two solutions of (3.3) is a multiple of the identity.

Theorem 3.2 ([8, Theorem 3.5]) *Consider an OQRW on a crystal lattice (embedded in $\mathbb{R}^d$). Assume that the hypothesis (H1) is satisfied. Let $(\rho_n, X_n)_{n\geq 0}$ be the quantum trajectory process associated with this OQRW. Then,*

$$\frac{X_n - nm}{\sqrt{n}}$$

converges in law to the Gaussian distribution $N(0, \Sigma)$ in $\mathbb{R}^d$, with covariance matrix $\Sigma = (C_{ij})_{i,j=1}^d$ given by

$$C_{ij} = -m_i m_j + \sum_{e\in A(G_0)} \mathrm{Tr}(B(e)\rho_\infty B(e)^*)(\widehat{\theta}(e))_i(\widehat{\theta}(e))_j$$
$$+2\sum_{e\in A(G_0)} \mathrm{Tr}(B(e)\rho_\infty B(e)^* L_{\mathbf{e}_i})(\widehat{\theta}(e))_j - 2m_i \mathrm{Tr}(\rho_\infty L_{\mathbf{e}_j}). \qquad (3.4)$$

Here, for $l \in \mathbb{R}^d$, L_l denotes the solution of the equation (3.3).

In [8], we gave some examples satisfying the CLT for the OQRWs on the hexagonal lattices. In "Appendix A," we give more examples of CLT for OQRWs on the triangular and Kagome lattices.

4 Mixture of Gaussians

In this section, we study the situation where the mixture of Gaussians occurs. Notice that the operator $\mathcal{L}_*$ in (3.1) is a generator for a (dual) quantum Markov semigroup. The hypothesis for the CLT in (H1) then says that the quantum Markov semigroup has a unique invariant state. Therefore, it is natural to ask what would be happening when there are multiple of invariant states for the quantum Markov semigroup. It is the main goal of this paper to investigate this situation. In the first subsection, we review the basic facts on the structure of invariant states for quantum Markov semigroup. In Sect. 4.2, we apply it to our model of OQRWs on the crystal lattices.

4.1 Structure of invariant states of quantum Markov semigroups on the finite-dimensional spaces

In this subsection, we recall some general theory of the structure of invariant states for the quantum Markov semigroups (QMSs) [4,6,11,12]. For the application to our model, it is enough to consider only the QMSs on the finite-dimensional spaces.

Let $\mathfrak{h}$ be a finite-dimensional Hilbert space. Let $\mathcal{A} := \mathcal{B}(\mathfrak{h})$, the space of all bounded linear operators on $\mathfrak{h}$, and consider the GKSL generator: for $H = H^*$, and $\{L_j\}$, the elements of $\mathcal{A}$,

$$\mathcal{L}(x) = i[H, x] - \frac{1}{2}\sum_j (L_j^* L_j x - 2L_j^* x L_j + x L_j^* L_j), \quad x \in \mathcal{A}. \qquad (4.1)$$

The dual generator is given by

$$\mathcal{L}_*(\rho) = -i[H, \rho] - \frac{1}{2}\sum_j (L_j^* L_j \rho - 2L_j \rho L_j^* + \rho L_j^* L_j), \quad \rho \in \mathcal{I}_1(\mathfrak{h}). \tag{4.2}$$

The state ρ is invariant for the QMS $\mathcal{T} = (\mathcal{T}_t)_{t\geq 0}$ with generator $\mathcal{L}$ if and only if $\mathcal{L}_*(\rho) = 0$.

Definition 4.1 ([11,12]) The projection $p_R := \sup\{p_i\}$, where the p_i's are the support projections of all invariant states of $\mathcal{T}$, is called the fast recurrent projection associated with a QMS $\mathcal{T}$.

A positive operator a is called subharmonic (resp. superharmonic, resp. harmonic) if $\mathcal{T}_t(a) \geq a$ (resp. $\mathcal{T}_t(a) \leq a$, resp. $\mathcal{T}_t(a) = a$) for all $t \geq 0$. It is known that the support projection of an invariant state for a QMS is subharmonic [4,11,12]. Moreover, the projection $p = \sup_{i\in I} p_i$, where $\{p_i\}_{i\in I}$ is a family of subharmonic projections for $\mathcal{T}$, is also subharmonic for $\mathcal{T}$, and hence, the fast recurrent projection p_R is subharmonic for $\mathcal{T}$.

If p is a subharmonic projection, one can define a reduced QMS associated with p, denoted by $(\mathcal{T}_t^p)_{t\geq 0}$, on $p\mathcal{A}p$ [11,12] by

$$\mathcal{T}_t^p(a) := p\mathcal{T}_t(a)p, \quad a \in p\mathcal{A}p, \ t \geq 0. \tag{4.3}$$

It was shown in [12] that when $\mathfrak{h}$ is of finite dimensional in particular, we have a decomposition

$$p_R \oplus p_T = I_{\mathfrak{h}},$$

where p_T is the transient projection associated with the QMS $\mathcal{T}$ (see [12] for the details). Moreover, we have for any $\varphi \in \mathcal{A}_*$,

$$\lim_{t\to\infty} \varphi(\mathcal{T}_t(p_T)) = 0.$$

(See [12, Corollary 2], [4, Proposition 6].)

Next, we discuss the invariant states for the QMSs. Recall that a QMS $\mathcal{T} = (\mathcal{T}_t)_{t\geq 0}$ is called irreducible if there is no non-trivial subharmonic projection [5]. Let us consider the following hypothesis [11]:

(H2) There is an orthonormal set $\{p_i\}_{i=1}^k$ of projections such that:

(a) $p_R = \sum_{i=1}^k p_i$;
(b) $\mathcal{T}_t^{p_R}(p_i) = p_i$ for all $i \in \{1, \cdots, k\}$;
(c) The restriction of $\mathcal{T}^{p_R}$ to the subalgebra $p_i\mathcal{A}p_i$ is irreducible for all $i \in \{1, \cdots, k\}$.

When $\mathfrak{h}$ is of finite dimensional, in particular, it was shown in [11,12] $p_R \neq 0$ and (H2) can be satisfied. From now on, we suppose that (H2) holds. In this case, the restriction of $\mathcal{T}^{p_R}$ to $p_i\mathcal{A}p_i$ is a reduced semigroup $\mathcal{T}^{p_i}$ for all i. For any state ω on $\mathcal{A}$ and a projection p, $p\omega p$ is a linear functional on $\mathcal{A}$ defined by $p\omega p(x) = \omega(pxp)$ [11]. Suppose that ω is a normal invariant state for the QMS and assume that $\omega(p_i) \neq 0$. As was observed in [11], the state $\rho_{i,\infty} := \omega(p_i)^{-1} p_i \omega p_i$ is a unique faithful and normal $\mathcal{T}^{p_i}$-invariant state on the subalgebra $p_i \mathcal{A} p_i$ (see Sect. 3.6.2 of [11]). By Theorem 3.7 of [11], $\mathcal{T}^{p_i}$ is mean ergodic, meaning that $\{t^{-1} \int_0^t \mathcal{T}_s^{p_i}(a)ds\}_{t>0}$ is weakly* convergent for every $a \in p_i \mathcal{A} p_i$. Suppose that μ is any state such that $s(\mu)$, the support of μ, satisfies $s(\mu) \leq p_i$ for some i. By [11, Theorem 3.13], we have

$$\text{w-}\lim_{t\to\infty} \frac{1}{t} \int_0^t \mathcal{T}_{*s}^{p_i}(\mu)ds = \rho_{i,\infty}.$$

We notice that any invariant state ω is a convex combination of $\rho_{i,\infty}$'s:

$$\omega = \sum_{i=1}^k \lambda_i \rho_{i,\infty}, \quad \sum_{i=1}^k \lambda_i = 1.$$

4.2 Mixture of Gaussians in OQRWs

We now consider the QMS in relevance with the OQRWs on the crystal lattices introduced in Sect. 2.2. The finite-dimensional Hilbert space is then $\mathfrak{h} = \oplus_{u\in V_0} \mathfrak{h}_u$. Let $\mathcal{T} = (\mathcal{T}_t)_{t\geq 0}$ be the QMS on $\mathcal{A} = \mathcal{B}(\mathfrak{h})$ with the (bounded) GKSL generator in (4.1) for $H = 0$ and $\{L_j\} = \{B(e)\}_{e\in A(G_0)}$. Since $\sum_e B(e)^* B(e) = I$, we have

$$\mathcal{L}(x) = \sum_{e\in A(G_0)} B(e)^* x B(e) - x, \quad x \in \mathcal{A}, \tag{4.4}$$

and the dual generator becomes

$$\mathcal{L}_*(\rho) = \sum_{e\in A(G_0)} B(e)\rho B(e)^* - \rho, \quad \rho \in \mathcal{A}_*. \tag{4.5}$$

As was noticed in the previous subsection, we have $I_{\mathfrak{h}} = p_R \oplus p_T$, where p_R and p_T are the fast recurrent and transient subspaces for $\mathcal{T}$, respectively. Let $\mathcal{M}$ be the OQRW in (2.7) on a crystal lattice $G = (V, A)$, which is a covering graph of $G_0 = (V_0, E_0)$. We assume that the hypothesis (H2) holds for the QMS on $\mathcal{A} = \mathcal{B}(\mathfrak{h})$ with GKSL generator in (4.4).

Lemma 4.2 *Under the hypothesis (H2), it holds that*

$$B(e)p_i = p_i B(e) p_i, \quad B(e)^* p_i = p_i B(e)^* p_i, \quad e \in A(V_0), \; i = 1, \cdots, k.$$

Proof It follows from [5, Theorem 5.7]. □

Let us define $B_i(e) := p_i B(e) p_i$, $i = 1, \cdots, k$, $e \in A(G_0)$. The reduced semigroup $\mathcal{T}^{p_i}$ is nothing but the QMS on $\mathcal{A}_i = p_i \mathcal{A} p_i$ with the GKSL generator given by

$$\mathcal{L}^{(i)}(x) = \sum_{e \in A(G_0)} B_i(e)^* x B_i(e) - x, \quad x \in \mathcal{A}_i. \tag{4.6}$$

Now, we know that the QMS $\mathcal{T}^{p_i}$ is irreducible and has a unique invariant faithful state $\rho_{i,\infty}$, i.e., the equation $\mathcal{L}_*^{(i)}(\rho_{i,\infty}) = 0$ holds, where

$$\mathcal{L}_*^{(i)}(\rho) := \sum_{e \in A(G_0)} B_i(e) \rho B_i(e)^* - \rho, \quad \rho \in p_i \mathcal{A}_* p_i. \tag{4.7}$$

For each $i = 1, \cdots, k$, let $\mathcal{M}^{(i)}$ be the OQRW defined on the crystal lattice $G = (V, A)$, which is defined by (2.7) with L_x^e's being replaced by

$$L_{i,x}^e := B_i(e) \otimes |x + \widehat{\theta}(e)\rangle\langle x|, \quad e \in A(G_0), \ x \in \mathbb{L}, \ i = 1, \cdots, k. \tag{4.8}$$

Now for each $i = 1, \cdots, k$, the generator $\mathcal{L}_*^{(i)}$ satisfies the hypothesis (H1). Therefore, by Theorem 3.2, the OQRW $\mathcal{M}^{(i)}$ with an initial condition $\rho^{(0)} = \rho_0 \otimes |0\rangle\langle 0|$ satisfying $s(\rho_0) \le p_i$ satisfies the CLT. Let us state it more in detail. For each $i = 1, \cdots, k$, define

$$m^{(i)} := \sum_{e \in A(G_0)} \mathrm{Tr}\left(B_i(e) \rho_{i,\infty} B_i(e)^*\right) \widehat{\theta}(e). \tag{4.9}$$

Also, for each $l \in \mathbb{R}^d$, let $L_l^{(i)}$ be a solution (which is unique up to a sum of a constant multiple of p_i) to the equation

$$-\mathcal{L}^{(i)}(L) = \sum_{e \in A(G_0)} B_i(e)^* B_i(e) \left(\widehat{\theta}(e) \cdot l\right) - (m^{(i)} \cdot l) p_i, \quad L \in \mathcal{A}_i. \tag{4.10}$$

Let $\Sigma^{(i)} = (C_{jl}^{(i)})_{j,l=1}^d$ be a covariance matrix whose elements are given by

$$\begin{aligned} C_{jl}^{(i)} &= -m_j^{(i)} m_l^{(i)} + \sum_{e \in A(G_0)} \mathrm{Tr}(B_i(e) \rho_{i,\infty} B_i(e)^*) (\widehat{\theta}(e))_j (\widehat{\theta}(e))_l \\ &\quad + 2 \sum_{e \in A(G_0)} \mathrm{Tr}(B_i(e) \rho_{i,\infty} B_i(e)^* L_{\mathbf{e}_j}^{(i)}) (\widehat{\theta}(e))_l - 2 m_j^{(i)} \mathrm{Tr}(\rho_{i,\infty} L_{\mathbf{e}_l}^{(i)}). \end{aligned} \tag{4.11}$$

Now, the CLT for $\mathcal{M}^{(i)}$ reads as follows.

Proposition 4.3 *Suppose that the hypothesis (H2) holds. Let $\mathcal{M}$ be an OQRW with an initial state $\rho^{(0)} = \rho_0 \otimes |0\rangle\langle 0|$ such that $s(\rho_0) \le p_i$ for some $i \in \{1, 2, \cdots, k\}$. Then, the position random variables $(X_n)_{n \ge 0}$ satisfy a CLT: As $n \to \infty$, $(X_n - n m^{(i)})/\sqrt{n}$ converges in law to a Gaussian distribution $N(0, \Sigma^{(i)})$, where the mean $m^{(i)}$ and covariance matrix $\Sigma^{(i)}$ are given in (4.9) and (4.11), respectively.*

Proof Since the subspace p_i is invariant for the QMS $\mathcal{T}^{(i)}$, the OQRW $\mathcal{M}$ becomes $\mathcal{M}^{(i)}$. For $\mathcal{M}^{(i)}$, the hypothesis (H1) holds and the statement follows from Theorem 3.2. □

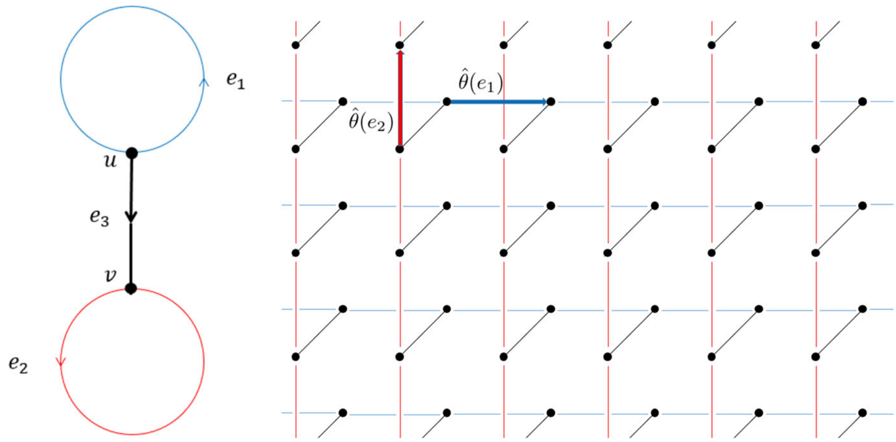

Fig. 3 $\mathbb{Z}^2$ with sites of intrinsic two points

The following is a main theorem of this paper.

Theorem 4.4 *Let us suppose that the hypothesis (H2) holds. Let* $\rho^{(0)} := \rho_0 \otimes |0\rangle\langle 0|$ *be an initial state for the OQRW such that*

$$\rho_0 = \sum_{i=1}^{k} \rho_{0,i},$$

where $s(\rho_{0,i}) \leq p_i$, $i = 1, \cdots, k$. *Let* $\lambda_i := \mathrm{Tr}(\rho_{0,i})$. *Then, with probability* λ_i, *the position random variables* $(X_n)_{n\in\mathbb{N}}$ *satisfy that as* $n \to \infty$, $(X_n - nm^{(i)})/\sqrt{n}$ *converges in law to a Gaussian distribution* $N(0, \Sigma^{(i)})$, *where the mean* $m^{(i)}$ *and covariance matrix* $\Sigma^{(i)}$ *are given in* (4.9) *and* (4.11), *respectively.*

Proof We can say that with probability λ_i the OQRW starts from an initial state $\frac{\rho_{0,i}}{\mathrm{Tr}(\rho_{0,i})} \otimes |0\rangle\langle 0|$. The conclusion follows from Proposition 4.3. □

Remark 4.5 A similar investigation was done in [1, Theorem 7.3]. There, it was shown that if the intrinsic Hilbert space (the space $\mathfrak{h}$ in the present notation) is a direct sum of some subspaces and moreover if the Kraus operators are invariant on each subspaces, i.e., they are of block diagonal form, then a mixture of Gaussians would appear in the limit (see [1, Section 7] for the details). However, no example was provided there.

4.3 Examples

4.3.1 $\mathbb{Z}^2$ with sites of intrinsic two points

Consider the two-dimensional integer lattice $\mathbb{Z}^2$, but whose sites consist of two intrinsic points. See Fig. 3. We let $V_0 = \{u, v\}$ and let $\{e_i\}_{i=1,2,3}$ be the three edges as shown in Fig. 3. Let

$$\widehat{\theta}(e_1) = [1, 0], \quad \widehat{\theta}(e_2) = [0, 1], \quad \widehat{\theta}(e_3) = 0,$$

and $\widehat{\theta}(\overline{e}_i) = -\widehat{\theta}(e_i)$, $i = 1, 2, 3$. In order to define the operators $B(e)$, $e \in A(G_0)$, let $\mathfrak{h}_u = \mathfrak{h}_v = \mathbb{C}^3$, and $\mathfrak{h} = \mathfrak{h}_u \oplus \mathfrak{h}_v \simeq \mathbb{C}^6$. Let $U = \begin{bmatrix}\mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3\end{bmatrix}$ and $V = \begin{bmatrix}\mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3\end{bmatrix}$ be 3×3 unitary matrices with column vectors $\mathbf{u}_i = [u_{1i}, u_{2i}, u_{3i}]^T$ and $\mathbf{v}_i = [v_{1i}, v_{2i}, v_{3i}]^T$, $i = 1, 2, 3$. For $i = 1, 2, 3$, let U_i be a 3×3 matrix whose ith column is $\mathbf{u}_i$ and remaining columns are zeros. Similarly, let V_i be the 3×3 matrix, whose ith column is the vector $\mathbf{v}_i$ and other columns are zeros. Let us define 6×6 matrices $B(e)$, $e \in A(G_0)$, whose block matrices are given as follows:

$$B(e_1) = \begin{bmatrix} U_1^* & 0 \\ 0 & 0 \end{bmatrix}, \quad B(\overline{e}_1) = \begin{bmatrix} U_2^* & 0 \\ 0 & 0 \end{bmatrix}, \quad B(e_3) = \begin{bmatrix} 0 & 0 \\ U_3^* & 0 \end{bmatrix},$$
$$B(e_2) = \begin{bmatrix} 0 & 0 \\ 0 & V_1^* \end{bmatrix}, \quad B(\overline{e}_2) = \begin{bmatrix} 0 & 0 \\ 0 & V_2^* \end{bmatrix}, \quad B(\overline{e}_3) = \begin{bmatrix} 0 & V_3^* \\ 0 & 0 \end{bmatrix}.$$

We easily check condition (2.4) holds. Then, the OQRW is defined by formula (2.7). **One model**. Let us take $U = V \equiv U_H$, where

$$U_H := \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{4.12}$$

It is not hard to check that the hypothesis (H2) is satisfied with $p_R = I_{\mathbb{C}^3 \oplus \mathbb{C}^3} = p_1 + p_2 + p_3$;

$$p_1 = (I_2 \oplus 0_1) \oplus 0_3, \quad p_2 = 0_3 \oplus (I_2 \oplus 0_1), \quad p_3 = (0_2 \oplus I_1) \oplus (0_2 \oplus I_1),$$

where I_d and 0_d mean the d-dimensional identity and zero matrices, respectively. The invariant states (density matrices) satisfying $\mathcal{L}_* = 0$ are

$$\rho_{1,\infty} = \frac{1}{2} p_1, \quad \rho_{2,\infty} = \frac{1}{2} p_2, \quad \rho_{3,\infty} = \frac{1}{2} p_3.$$

We can easily compute the means $m^{(i)}$ and covariance matrices $\Sigma^{(i)}$, $i = 1, 2, 3$, by formulas (4.9) and (4.11), respectively, to get

$$m^{(1)} = m^{(2)} = m^{(3)} = 0, \text{ and } \Sigma^{(1)} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \Sigma^{(2)} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad \Sigma^{(3)} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

For $i = 1, 2, 3$, let $\mu^{(i)}$ be the two-dimensional Gaussian distributed as $N(0, \Sigma^{(i)})$. By Theorem 4.4, for an initial state $\rho^{(0)} = \rho_0 \otimes |0\rangle\langle 0|$ such that $\rho_0 = \sum_{i=1}^{3} \rho_{0,i}$ with

$s(\rho_{0,i}) \leq p_i$, $i = 1, 2, 3$, the OQRW on the crystal lattice $\mathbb{Z}^2$ with sites of intrinsic two points satisfies as $n \to \infty$

$$\frac{X_n}{\sqrt{n}} \xrightarrow{(\mathrm{d})} \sum_{i=1}^{3} \lambda_i \mu^{(i)},$$

where $\lambda_i = \mathrm{Tr}(\rho_{0,i})$, $i = 1, 2, 3$.

Another model This time let us take $U = U_H$ in (4.12) and $V = U_G$, where

$$U_G := \frac{1}{3}\begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}. \tag{4.13}$$

We can check that the hypothesis (H2) is satisfied with $p_R = I_{\mathbb{C}^3 \oplus \mathbb{C}^3} = p_1 + p_2$;

$$p_1 = (I_2 \oplus 0_1) \oplus 0_3, \quad p_2 = (0_2 \oplus I_1) \oplus I_3.$$

The invariant states (density matrices) satisfying $\mathcal{L}_* = 0$ are

$$\rho_{1,\infty} = \frac{1}{2} p_1 \text{ and } \rho_{2,\infty} = \frac{1}{4} p_2.$$

We can compute the means $m^{(i)}$ and covariance matrices $\Sigma^{(i)}$, $i = 1, 2$, by formulas (4.9) and (4.11), respectively. First, we easily see that $m^{(1)} = m^{(2)} = 0$. By directly solving equation (4.10), we get

$$L_{\mathbf{e}_1}^{(1)} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad L_{\mathbf{e}_2}^{(1)} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix},$$
$$L_{\mathbf{e}_1}^{(2)} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad L_{\mathbf{e}_2}^{(2)} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -1/4 & 0 & -1/2 \\ 0 & 0 & 1/4 & 1/2 \\ 0 & -1/2 & 1/2 & 0 \end{bmatrix},$$

up to a sum of constant multiples of p_i for $i = 1, 2$, respectively. Computing the covariances from (4.11), we get

$$\Sigma^{(1)} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \text{ and } \Sigma^{(2)} = \begin{bmatrix} 0 & 0 \\ 0 & 1/4 \end{bmatrix}.$$

Therefore, as in the previous example, for an initial state $\rho^{(0)} = \rho_0 \otimes |0\rangle\langle 0|$ such that $\rho_0 = \sum_{i=1}^{2} \rho_{0,i}$ with $s(\rho_{0,i}) \leq p_i$, $i = 1, 2$, the OQRW in this model satisfies as $n \to \infty$

$$\frac{X_n}{\sqrt{n}} \xrightarrow{(\mathrm{d})} \sum_{i=1}^{2} \lambda_i \mu^{(i)},$$

where $\lambda_i = \text{Tr}(\rho_{0,i})$, and $\mu^{(i)}$ is the two-dimensional Gaussian distributed as $N(0, \Sigma^{(i)})$ for $i = 1, 2$. Here, we may notice that the variance in the p_2-subsystem is smaller than the one in the p_1-subsystem because there is an idling in the former one, meaning that the walker may stay at the present place without jump, and it results in the slow spread giving a smaller variance.

4.3.2 Hexagonal lattice

Next, we consider another example on the hexagonal lattice. See Fig. 1. The central limit theorems for this model were widely studied in [8]. Let us recall some notions introduced there. We let $V_0 = \{u, v\}$ and let $\{e_i\}_{i=1,2,3}$ be the three edges in G_0 with $\text{o}(e_i) = u$ and $\text{t}(e_i) = v$. (See Fig. 1.) The reversed edges are $\overline{e}_i$, $i = 1, 2, 3$. We let

$$\widehat{\theta}(e_1) = \frac{1}{\sqrt{2}}[1, 1], \quad \widehat{\theta}(e_2) = \frac{1}{\sqrt{2}}[-1, 1], \quad \widehat{\theta}(e_3) = 0,$$

and $\widehat{\theta}(\overline{e}_i) = -\widehat{\theta}(e_i)$, $i = 1, 2, 3$. Similar to the previous example, let $\mathfrak{h}_u = \mathfrak{h}_v = \mathbb{C}^3$, and $\mathfrak{h} = \mathfrak{h}_u \oplus \mathfrak{h}_v \simeq \mathbb{C}^6$. Let $U = \begin{bmatrix}\mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3\end{bmatrix}$ and $V = \begin{bmatrix}\mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3\end{bmatrix}$ be 3×3 unitary matrices with column vectors $\mathbf{u}_i = [u_{1i}, u_{2i}, u_{3i}]^T$ and $\mathbf{v}_i = [v_{1i}, v_{2i}, v_{3i}]^T$, $i = 1, 2, 3$. For $i = 1, 2, 3$, let U_i be a 3×3 matrix whose ith column is $\mathbf{u}_i$ and remaining columns are zeros. Similarly, let V_i be the 3×3 matrix, whose ith column is the vector $\mathbf{v}_i$ and other columns are zeros. Now for $i = 1, 2, 3$, let $\widetilde{U}_i$ and $\widetilde{V}_i$ be 6×6 matrices whose block matrices are given as follows:

$$\widetilde{U}_i = \begin{bmatrix} 0 & 0 \\ U_i & 0 \end{bmatrix}, \quad \widetilde{V}_i = \begin{bmatrix} 0 & V_i \\ 0 & 0 \end{bmatrix}.$$

We define

$$B(e_i) := \widetilde{U}_i, \quad \text{and} \quad B(\overline{e}_i) := \widetilde{V}_i, \quad i = 1, 2, 3.$$

We check again condition (2.4) holds. Then, the OQRW on the hexagonal lattice is defined by formula (2.7).

Recall the stochastic matrices P_U and P_V introduced in (A.2). The following proposition says that whether the limit behavior of OQRWs on the hexagonal lattice satisfies a Gaussian or a mixture of Gaussians, it is characterized by the form of the products $P_U P_V$ and $P_V P_U$.

Proposition 4.6 *If the stochastic matrices $P_U P_V$ and $P_V P_U$ are irreducible, then the equation $\mathcal{L}_*(\rho) = 0$ has a unique solution on the states; thereby, the central limit theorem holds. On the other hand, if $P_U P_V$ and $P_V P_U$ are reducible with a common decomposition into communicating classes, then the hypothesis (H2) is satisfied and Theorem 4.4 applies resulting in the mixture of Gaussians.*

The proof of uniqueness and nonuniqueness for the equation $\mathcal{L}_* = 0$ according to the conditions mentioned in the proposition was shown in [8, Proposition 4.1]. By the proof there, if $P_U P_V$ and $P_V P_U$ are reducible with a common decomposition $\{1, 2, 3\} = \{\{1, 2\}, \{3\}\}$ into communicating classes (we take $\{1, 2, 3\}$ as the state space for the classical Markov chain), for example, then we have

$$p_R = I_{\mathfrak{h}} = p_1 + p_2,$$

with

$$p_1 = (I_2 \oplus 0_1) \oplus (I_2 \oplus 0_1) \text{ and } p_2 = (0_2 \oplus I_1) \oplus (0_2 \oplus I_1),$$

where I_d and 0_d mean again the identity and zero operator on $\mathbb{C}^d$, respectively. Moreover, the invariant states for each subspaces are

$$\rho_{1,\infty} = \frac{1}{4} p_1 \text{ and } \rho_{2,\infty} = \frac{1}{2} p_2.$$

Let us take some concrete examples. First, for CLT, let us take $U = V = U_G$ in (4.13). In this case since

$$P_U P_V = P_V P_U = \frac{1}{81} \begin{bmatrix} 33 & 24 & 24 \\ 24 & 33 & 24 \\ 24 & 24 & 33 \end{bmatrix},$$

Proposition 4.6 says that the central limit theorem holds. The concrete computation of the mean and covariance for this model was done in [8, Subsection 4.2]. Next, we take $U = V = U_H$ given in (4.12). In this case, we have

$$P_U = P_V = \frac{1}{2} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}, \tag{4.14}$$

and hence, a mixture of Gaussians appears in the limit of the OQRWs. With some computations, one can show the mean and covariance for each subsystem:

$$m^{(1)} = m^{(2)} = 0, \text{ and } \Sigma^{(1)} = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \ \Sigma^{(2)} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

For $i = 1, 2$, let $\mu^{(i)}$ be the Gaussians distributed as $N(0, \Sigma^{(i)})$ ($\mu^{(2)} = \delta_0$, in fact). Then by Theorem 4.4, for an initial state $\rho^{(0)} = \rho_0 \otimes |0\rangle\langle 0|$ such that $\rho_0 = \sum_{i=1}^{2} \rho_{0,i}$ with $s(\rho_{0,i}) \le p_i$, $i = 1, 2$, the OQRW in this model satisfies as $n \to \infty$

$$\frac{X_n}{\sqrt{n}} \xrightarrow{\text{(d)}} \lambda \mu^{(1)} + (1 - \lambda) \mu^{(2)},$$

where $\lambda = \mathrm{Tr}(\rho_{0,1})$. In "Appendix B," we check this result by an analytic method using Fourier transforms.

5 Discussion

We have investigated when a mixture of Gaussians appears in the limit distribution of the OQRWs. It depends whether the intrinsic QMS, whose GKSL generator comes from the Kraus operators of the OQRW, has multiple invariant states or not. We concretely considered some models on the crystal lattices. We have provided not only examples of CLT but also examples of a mixture of Gaussians. The crystal lattices we considered are $\mathbb{Z}^2$ with intrinsic points, the hexagonal, triangular, and Kagome lattices.

In order to investigate the general limit theorems, we reviewed the structure of the invariant states for QMS. For finite dimension QMSs, we can have models in which the invariant subspaces are orthogonal to each other. For the applications to the OQRWs, we particularly consider the GKSL generators coming from the Kraus operators for OQRWs. Some concrete models are constructed on $\mathbb{Z}^2$ with intrinsic two points as well as on the hexagonal lattices.

In "Appendix A," we consider some further models for CLT for OQRWs on the triangular and Kagome lattices. It serves as supplementary models to the one discussed in [8], where the CLT for OQRWs on the hexagonal lattices was presented. For the model on the triangular lattice, we may say that the walk is not of the nearest neighbor jumps in the two-dimensional lattice. The nearest jumps are to move by $\pm\widehat{\theta}_1$ or $\pm\widehat{\theta}_2$, where $\widehat{\theta}_1 = \frac{1}{\sqrt{2}}[1,1]^T$ and $\frac{1}{\sqrt{2}}[-1,1]^T$. But, it is possible for the walker to jump to $\pm(\widehat{\theta}_1+\widehat{\theta}_2) = \pm\sqrt{2}[0,1]^T$. This effect gives a bigger variance in the y-direction. See (A.7). For the Kagome lattice, we have constructed a simplest example showing Gaussian limit. Since the structure of Kagome lattice is rather complex comparing with triangular or hexagonal lattices, it is much harder to check the uniqueness of the invariant state for the Markov generator (3.1). (See Lemma A.1.) However, it leaves us with many rooms to construct different kinds of walks.

In Appendix B, we introduce another method to get limit theorems for OQRWs, namely the Fourier analysis developed in [8]. We see that the two different methods give the same results.

Finally, we would like to mention an open problem. The main result Theorem 4.4 and the examples that follow deal with the initial states of block diagonal form, i.e., direct sum of restrictions whose supports are smaller than the corresponding subharmonic projections. The most general result would be the knowledge on the limit distributions for arbitrary initial conditions.

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A Examples: central limit theorem

In this Appendix, we consider some more examples satisfying the CLT. The examples of OQRWs on the hexagonal lattice were investigated in [8]. Here, we consider the examples for the triangular and Kagome lattices.

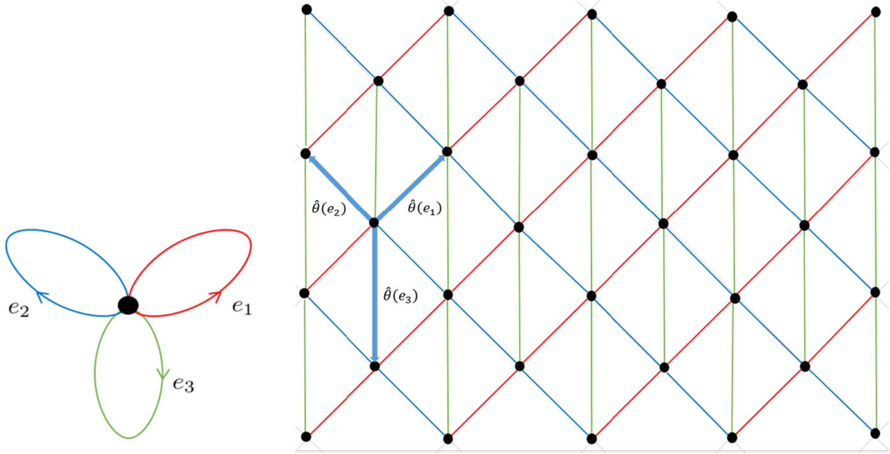

Fig. 4 Triangular lattice

A.1 Triangular lattice

Triangular lattice is a crystal lattice that is depicted in $\mathbb{R}^2$. Look at Figure 4.

A.1.1 Preparation

We let $V_0 = \{u\}$ and let $\{e_i\}_{i=1,2,3}$ be the three self-loops in G_0 with $\mathrm{o}(e_i) = \mathrm{t}(e_i) = u$. (See Figure 4.) The reversed self-loops are denoted by $\overline{e}_i$, $i = 1, 2, 3$. It is natural to define $\mathfrak{h} \equiv \mathfrak{h}_u = \mathbb{C}^6$ and find six matrices $B(e)$, $e \in A(G_0)$, of size 6×6 that satisfy (2.4). However, it is too much to investigate all the general cases. Here, we focus on the simple examples that satisfy the central limit theorems. For that, we let $\mathfrak{h} = \mathbb{C}^3 \oplus \mathbb{C}^3$ and consider 3×3 block matrices for $B(e)$, $e \in A(G_0)$, as follows. We remark that the following construction is very similar to the example for hexagonal lattice studied in [8]. First, we let

$$\widehat{\theta}(e_1) = \frac{1}{\sqrt{2}}[1, 1], \quad \widehat{\theta}(e_2) = \frac{1}{\sqrt{2}}[-1, 1], \quad \widehat{\theta}(e_3) = [0, -\sqrt{2}],$$

and $\widehat{\theta}(\overline{e}_i) = -\widehat{\theta}(e_i)$, $i = 1, 2, 3$. In order to define the operators $B(e)$, $e \in A(G_0)$, let $U = \begin{bmatrix}\mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3\end{bmatrix}$ and $V = \begin{bmatrix}\mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3\end{bmatrix}$ be 3×3 unitary matrices with column vectors $\mathbf{u}_i = [u_{1i}, u_{2i}, u_{3i}]^T$ and $\mathbf{v}_i = [v_{1i}, v_{2i}, v_{3i}]^T$, $i = 1, 2, 3$. For $i = 1, 2, 3$, let U_i be a 3×3 matrix whose ith column is $\mathbf{u}_i$ and the remaining columns are zeros. Similarly, let V_i be the 3×3 matrix, whose ith column is the vector $\mathbf{v}_i$ and other columns are zeros. For $i = 1, 2, 3$, let $\widetilde{U}_i$ and $\widetilde{V}_i$ be 6×6 matrices whose block matrices are given as follows:

$$\widetilde{U}_i = \begin{bmatrix} 0 & 0 \\ U_i & 0 \end{bmatrix}, \quad \widetilde{V}_i = \begin{bmatrix} 0 & V_i \\ 0 & 0 \end{bmatrix}.$$

Now, we define

$$B(e_i) := \widetilde{U}_i, \quad \text{and} \quad B(\overline{e}_i) := \widetilde{V}_i, \quad i = 1, 2, 3.$$

Then, $B(e_i),\ B(\overline{e}_i),\ i = 1, 2, 3$ satisfy condition (2.4).

It is easy to check that a state $\rho \in \mathcal{E}(\mathfrak{h})$ is a solution to the equation $\mathcal{L}_*(\rho) = 0$, where $\mathcal{L}_*(\rho)$ was defined in (3.1), if and only if $\rho = \rho_1 \oplus \rho_2$ and it holds that

$$\rho_1 = \sum_{i=1}^{3} V_i \rho_2 V_i^*, \qquad \rho_2 = \sum_{i=1}^{3} U_i \rho_1 U_i^*. \tag{A.1}$$

Let us consider the following (doubly) stochastic matrices:

$$P_U := \begin{bmatrix} |u_{11}|^2 & |u_{21}|^2 & |u_{31}|^2 \\ |u_{12}|^2 & |u_{22}|^2 & |u_{32}|^2 \\ |u_{13}|^2 & |u_{23}|^2 & |u_{33}|^2 \end{bmatrix}, \quad P_V := \begin{bmatrix} |v_{11}|^2 & |v_{21}|^2 & |v_{31}|^2 \\ |v_{12}|^2 & |v_{22}|^2 & |v_{32}|^2 \\ |v_{13}|^2 & |v_{23}|^2 & |v_{33}|^2 \end{bmatrix}. \tag{A.2}$$

It was shown in [8, Proposition 4.1] that if the stochastic matrices $P_U P_V$ and $P_V P_U$ are irreducible, then the equation $\mathcal{L}_*(\rho) = 0$ has a unique state solution $\rho = \rho_1 \oplus \rho_2$ with $\rho_1 = \rho_2 = \frac{1}{6} I$.

Example: nonzero covariance

Let us take $U = V = U_G$, where

$$U_G = \frac{1}{3} \begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}. \tag{A.3}$$

It is obvious that $P_U P_V = P_V P_U$ is irreducible, where P_U and P_V are defined in (A.2). Therefore, the equation $\mathcal{L}_*(\rho) = 0$ has a unique state solution $\rho = \frac{1}{6} I \oplus \frac{1}{6} I$. From equation (3.2), it is easy to see that $m = 0$. By directly computing from (3.3), we get, up to a sum of a constant multiple of identity,

$$L_1 = L_{1,u} \oplus L_{1,v}, \quad L_{1,u} = \begin{bmatrix} 3 & 0 & 0 \\ 0 & \frac{3}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad L_{1,v} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

and

$$L_2 = L_{2,u} \oplus L_{2,v}, \quad L_{2,u} = \begin{bmatrix} \frac{3}{2} & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad L_{2,v} = \begin{bmatrix} \frac{3}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 3 \end{bmatrix}.$$

Notice that the transformation matrix Θ in (2.1) is given by

$$\Theta = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}. \tag{A.4}$$

By the linearity of equation (3.3), we have (see [8, Remark 3.6])

$$L_{\mathbf{e}_i} = \sum_{j=1}^{2} \Theta_{ij} L_j, \quad i = 1, 2. \tag{A.5}$$

Therefore, we get

$$L_{\mathbf{e}_1} = \Theta_{11} L_1 + \Theta_{12} L_2 = L_{\mathbf{e}_1,1} \oplus L_{\mathbf{e}_1,2}, \quad L_{\mathbf{e}_1,1} = -L_{\mathbf{e}_1,2} = \frac{3}{2\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and

$$L_{\mathbf{e}_2} = \Theta_{21} L_1 + \Theta_{22} L_2 = L_{\mathbf{e}_2,1} \oplus L_{\mathbf{e}_2,2}$$

with

$$L_{\mathbf{e}_2,1} = \frac{9}{2\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad L_{\mathbf{e}_2,2} = \frac{3}{2\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 4 \end{bmatrix}.$$

Now, we are ready to compute the covariance matrix Σ given in (3.4). Since the mean m is zero and $\rho_\infty = \frac{1}{6} I$, we are left with

$$\begin{aligned} C_{ij} &= \frac{1}{6} \sum_{e \in A(G_0)} \mathrm{Tr}(B(e)B(e)^*)(\widehat{\theta}(e))_i (\widehat{\theta}(e))_j \\ &\quad + \frac{1}{3} \sum_{e \in A(G_0)} \mathrm{Tr}(B(e)B(e)^* L_{\mathbf{e}_i})(\widehat{\theta}(e))_j \\ &=: C_{ij}^{(1)} + C_{ij}^{(2)}. \end{aligned} \tag{A.6}$$

For the first term $C_{ij}^{(1)}$, the trace part is all 1 and thus we get

$$C^{(1)} = \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & 1 \end{bmatrix}.$$

For the second term $C_{ij}^{(2)}$, computations before taking trace give us

$$\sum_{e\in A(G_0)} (B(e)B(e)^*)(\widehat{\theta}(e))_j = \begin{cases} \frac{1}{3\sqrt{2}}\left(\begin{bmatrix}1 & 0 & 2\\ 0 & -1 & -2\\ 2 & -2 & 0\end{bmatrix} \oplus \begin{bmatrix}-1 & 0 & -2\\ 0 & 1 & 2\\ -2 & 2 & 0\end{bmatrix}\right), & j=1,\\ \frac{1}{3\sqrt{2}}\left(\begin{bmatrix}1 & 4 & -2\\ 4 & 1 & -2\\ -2 & -2 & -2\end{bmatrix} \oplus \begin{bmatrix}-1 & -4 & 2\\ -4 & -1 & 2\\ 2 & 2 & 2\end{bmatrix}\right), & j=2,\end{cases}$$

and so we get

$$C^{(2)} = \begin{bmatrix}\frac{1}{3} & 0\\ 0 & 1\end{bmatrix}.$$

Thus, summing those two terms we get the covariance matrix

$$\Sigma = C^{(1)} + C^{(2)} = 2\begin{bmatrix}\frac{1}{3} & 0\\ 0 & 1\end{bmatrix}. \tag{A.7}$$

The characteristic function for the Gaussian random variable X with mean zero and covariance Σ in (A.7) is

$$\mathbb{E}(e^{i\langle \mathbf{t}, X\rangle}) = e^{-\frac{1}{3}(t_1^2+3t_2^2)}.$$

We notice that the variance in the horizontal line (x-axis) is smaller than that in the vertical line (y-axis). This reflects that fact that along the vertical line there are "roads" (the vectors $\widehat{\theta}(e_3)$ and $\widehat{\theta}(\overline{e}_3)$) through which the walker can travel.

Example: zero covariance

Let us consider one more example for the model of OQRW on the triangular lattice. This time, let us take $U = U_G$ in (A.3) and $V = I$. In this case, the matrices $P_U P_V$ and $P_V P_U$ are also irreducible and hence the equation $\mathcal{L}_*(\rho) = 0$ has a unique state solution $\rho_\infty = \frac{1}{6}I$. From equation (3.2), it is easy to see that $m = 0$. As before, the solutions of (3.3) are, up to a sum of constant multiple of identity,

$$L_1 = L_{1,u} \oplus L_{1,v}, \quad L_{1,u} = \begin{bmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{bmatrix}, \ L_{1,v} = 0,$$

and

$$L_2 = L_{2,u} \oplus L_{2,v}, \quad L_{2,u} = \begin{bmatrix}0 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{bmatrix}, \ L_{2,v} = 0.$$

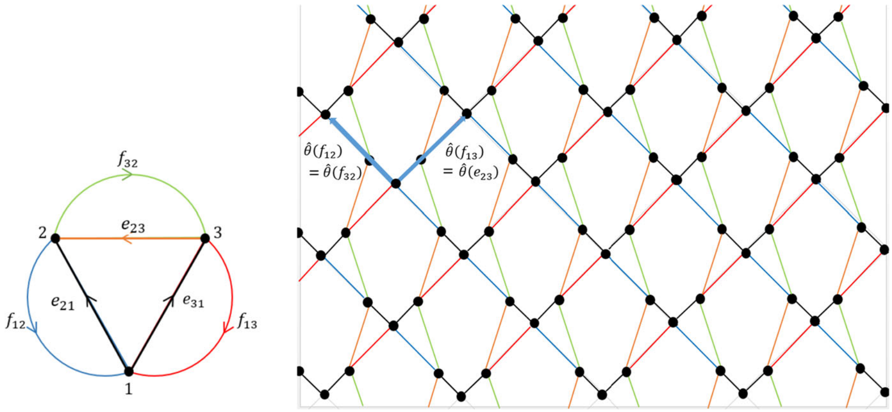

Fig. 5 Kagome lattice

Recall Θ in (A.4). We then get

$$L_{\mathbf{e}_1} = \Theta_{11}L_1 + \Theta_{12}L_2 = L_{\mathbf{e}_1,u} \oplus L_{\mathbf{e}_1,v}, \quad L_{\mathbf{e}_1,u} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad L_{\mathbf{e}_1,v} = 0,$$

and

$$L_{\mathbf{e}_2} = \Theta_{21}L_1 + \Theta_{22}L_2 = L_{\mathbf{e}_2,u} \oplus L_{\mathbf{e}_2,v}, \quad L_{\mathbf{e}_2,u} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}, \quad L_{\mathbf{e}_2,v} = 0.$$

The covariance matrix can be computed as before, and we get $\Sigma = 0$. Now, the measure is a Gaussian and the mean and covariance are all zero; this means that it is a Dirac measure at the origin.

A.2 Kagome lattice

In this subsection, we consider the OQRWs on the Kagome lattice. Look at the Kagome lattice in Fig. 5.

We let $V_0 = \{1, 2, 3\}$ by naming the vertices with numbers. For $1 \le i \ne j \le 3$, we let $\{e_{ij}, f_{ij}\}$ be the 12 directed edges in G_0 with a convention $\mathrm{o}(e_{ij}) = j$ and $\mathrm{t}(e_{ij}) = i$ and similarly for f_{ij}'s. We notice that $\overline{e}_{ij} = e_{ji}$ and $\overline{f}_{ij} = f_{ji}$. We let

$$\begin{aligned} \widehat{\theta}(e_{12}) = \widehat{\theta}(e_{21}) = \widehat{\theta}(e_{13}) = \widehat{\theta}(e_{31}) = 0, \\ \widehat{\theta}(e_{23}) = \widehat{\theta}(f_{13}) = -\widehat{\theta}(e_{32}) = -\widehat{\theta}(f_{31}) = \frac{1}{\sqrt{2}}[1, 1], \end{aligned}$$

and

$$\widehat{\theta}(f_{12}) = \widehat{\theta}(f_{32}) = -\widehat{\theta}(f_{21}) = -\widehat{\theta}(f_{23}) = \frac{1}{\sqrt{2}}[-1, 1].$$

In order to define the operators $B(e)$, $e \in A(G_0)$, let $\mathfrak{h}_1 = \mathfrak{h}_2 = \mathfrak{h}_3 = \mathbb{C}^4$, and $\mathfrak{h} = \mathfrak{h}_1 \oplus \mathfrak{h}_2 \oplus \mathfrak{h}_3 = \mathbb{C}^{12}$. Let H be a 2×2 unitary matrix given by

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} =: L + R,$$

where

$$L := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix}, \quad R := \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}.$$

Notice that

$$L^*L = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} =: P_1, \quad R^*R = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} =: P_2,$$
$$LL^* = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad RR^* = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}.$$

Let U_L, U_R, V_L, and V_R be 4×4 matrices given by

$$U_L = \begin{bmatrix} 0 & 0 \\ L & 0 \end{bmatrix}, \quad U_R = \begin{bmatrix} 0 & 0 \\ R & 0 \end{bmatrix}, \quad V_L = \begin{bmatrix} 0 & L \\ 0 & 0 \end{bmatrix}, \quad V_R = \begin{bmatrix} 0 & R \\ 0 & 0 \end{bmatrix}.$$

Notice that

$$U_L^*U_L = \begin{bmatrix} P_1 & 0 \\ 0 & 0 \end{bmatrix}, \quad U_R^*U_R = \begin{bmatrix} P_2 & 0 \\ 0 & 0 \end{bmatrix},$$
$$V_L^*V_L = \begin{bmatrix} 0 & 0 \\ 0 & P_1 \end{bmatrix}, \quad V_R^*V_R = \begin{bmatrix} 0 & 0 \\ 0 & P_2 \end{bmatrix}.$$

For $i, j = 1, 2, 3$ $(i \neq j)$, let U_{ij} and V_{ij} be 12×12 matrices whose block matrices are given as follows:

$$U_{21} = \begin{bmatrix} 0 & 0 & 0 \\ U_L & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad U_{31} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ U_R & 0 & 0 \end{bmatrix}, \quad U_{32} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & U_L & 0 \end{bmatrix},$$
$$U_{12} = \begin{bmatrix} 0 & U_R & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad U_{13} = \begin{bmatrix} 0 & 0 & U_L \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad U_{23} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & U_R \\ 0 & 0 & 0 \end{bmatrix},$$

and

$$V_{21} = \begin{bmatrix} 0 & 0 & 0 \\ V_L & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad V_{31} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ V_R & 0 & 0 \end{bmatrix}, \quad V_{32} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & V_L & 0 \end{bmatrix},$$
$$V_{12} = \begin{bmatrix} 0 & V_R & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad V_{13} = \begin{bmatrix} 0 & 0 & V_L \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad V_{23} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & V_R \\ 0 & 0 & 0 \end{bmatrix}.$$

Now, we define

$$B(e_{ij}) := U_{ij} \quad \text{and} \quad B(f_{ij}) := V_{ij}, \quad i = 1, 2, 3 \ (i \neq j).$$

Then, $B(e_{ij}),\ B(f_{ij}),\ i, j = 1, 2, 3\ (i \neq j)$ satisfy condition (2.4).

Lemma A.1 *The equation $\mathcal{L}_*(\rho) = 0$ for the states, where $\mathcal{L}_*(\rho)$ was defined in (3.1), has a unique solution $\rho_\infty = \frac{1}{12} I \oplus \frac{1}{12} I \oplus \frac{1}{12} I \in \mathcal{E}(\mathfrak{h})$.*

Proof It is easy to check that a state $\rho \in \mathcal{E}(\mathfrak{h})$ solves the equation $\mathcal{L}_*(\rho) = 0$ if and only if it has the form $\rho = \rho^{(1)} \oplus \rho^{(2)} \oplus \rho^{(3)}$ and satisfies

$$\begin{aligned} \rho^{(1)} &= U_R \rho^{(2)} U_R^* + V_R \rho^{(2)} V_R^* + U_L \rho^{(3)} U_L^* + V_L \rho^{(3)} V_L^*, \\ \rho^{(2)} &= U_R \rho^{(3)} U_R^* + V_R \rho^{(3)} V_R^* + U_L \rho^{(1)} U_L^* + V_L \rho^{(1)} V_L^*, \\ \rho^{(3)} &= U_R \rho^{(1)} U_R^* + V_R \rho^{(1)} V_R^* + U_L \rho^{(2)} U_L^* + V_L \rho^{(2)} V_L^*. \end{aligned} \tag{A.8}$$

From equations (A.8), we see that the matrices $\rho^{(i)}$, $i = 1, 2, 3$, are block matrices of the form

$$\rho^{(i)} = \begin{bmatrix} \rho_1^{(i)} & 0 \\ 0 & \rho_2^{(i)} \end{bmatrix}, \quad i = 1, 2, 3; \tag{A.9}$$

here, $\rho_j^{(i)}$, $j = 1, 2$, are 2×2 matrices, say

$$\rho_j^{(i)} := \begin{bmatrix} \rho_j^{(i)}(1,1) & \rho_j^{(i)}(1,2) \\ \rho_j^{(i)}(2,1) & \rho_j^{(i)}(2,2) \end{bmatrix}.$$

Using the form in (A.9), we can rewrite (A.8) in the following form:

$$\rho = S \rho S^*, \tag{A.10}$$

where ρ and S are 12×12 block matrices defined by

$$\rho = \begin{bmatrix} \rho_1^{(1)} & 0 & 0 & 0 & 0 & 0 \\ 0 & \rho_2^{(1)} & 0 & 0 & 0 & 0 \\ 0 & 0 & \rho_1^{(2)} & 0 & 0 & 0 \\ 0 & 0 & 0 & \rho_2^{(2)} & 0 & 0 \\ 0 & 0 & 0 & 0 & \rho_1^{(3)} & 0 \\ 0 & 0 & 0 & 0 & 0 & \rho_2^{(3)} \end{bmatrix}, \quad S = \begin{bmatrix} 0 & 0 & 0 & R & 0 & L \\ 0 & 0 & R & 0 & L & 0 \\ 0 & L & 0 & 0 & 0 & R \\ L & 0 & 0 & 0 & R & 0 \\ 0 & R & 0 & L & 0 & 0 \\ R & 0 & L & 0 & 0 & 0 \end{bmatrix}. \tag{A.11}$$

It is easy to check that S is a unitary matrix. Therefore, by multiplying S^* and S from left and right, respectively, to equation (A.10) we also have

$$\rho = S^* \rho S. \tag{A.12}$$

From (A.12), we see that $\rho_j^{(i)}$ are diagonal matrices:

$$\rho_j^{(i)} := \begin{bmatrix} \rho_j^{(i)}(1,1) & 0 \\ 0 & \rho_j^{(i)}(2,2) \end{bmatrix}, \quad i = 1, 2, 3, \quad j = 1, 2. \tag{A.13}$$

Now equating the first block in (A.10) and (A.12), we get

$$\rho_1^{(1)} = R\rho_2^{(2)} R^* + L\rho_2^{(3)} L^* = L^* \rho_2^{(2)} L + R^* \rho_2^{(3)} R,$$

or

$$\begin{bmatrix} \rho_1^{(1)}(1,1) & 0 \\ 0 & \rho_1^{(1)}(2,2) \end{bmatrix} = \frac{1}{2}\rho_2^{(2)}(2,2) \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \frac{1}{2}\rho_2^{(3)}(1,1) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{A.14}$$

$$= \frac{1}{2} \begin{bmatrix} \rho_2^{(2)}(1,1) + \rho_2^{(2)}(2,2) & 0 \\ 0 & \rho_2^{(3)}(1,1) + \rho_2^{(3)}(2,2) \end{bmatrix}. \tag{A.15}$$

Looking at the off-diagonal components, we get

$$\rho_2^{(2)}(2,2) = \rho_2^{(3)}(1,1).$$

Applying this relation to (A.15) and (A.14), we easily get

$$\rho_1^{(1)}(1,1) = \rho_2^{(2)}(2,2) = \rho_2^{(3)}(1,1) = \rho_1^{(1)}(2,2) = \rho_2^{(2)}(1,1) = \rho_2^{(3)}(2,2).$$

That is, $\rho_1^{(1)} = \rho_2^{(2)} = \rho_2^{(3)}$. Using the cyclic symmetry, we obtain that all six matrices $\rho_j^{(i)}$, $i = 1, 2, 3$, $j = 1, 2$, are the same to each other. Taking into account that ρ is a state, we conclude $\rho = \frac{1}{12}I \oplus \frac{1}{12}I \oplus \frac{1}{12}I \in \mathcal{E}(\mathfrak{h})$ and the proof is completed. □

Let us compute the mean m and covariance matrix Σ. From equation (3.2), it is easy to see that $m = 0$. By directly computing from (3.3), we see that, up to a sum of a constant multiple of identity,

$$L_1 = \begin{bmatrix} 1&0&0&0\\ 0&1&0&0\\ 0&0&0&0\\ 0&0&0&0 \end{bmatrix} \oplus \begin{bmatrix} 0&0&0&0\\ 0&0&0&0\\ 0&0&1&0\\ 0&0&0&1 \end{bmatrix} \oplus \begin{bmatrix} 0&0&0&0\\ 0&2&0&0\\ 0&0&2&0\\ 0&0&0&0 \end{bmatrix},$$

and

$$L_2 = \begin{bmatrix} 3&0&0&0\\ 0&1&0&0\\ 0&0&0&0\\ 0&0&0&2 \end{bmatrix} \oplus \begin{bmatrix} 1&0&0&0\\ 0&1&0&0\\ 0&0&3&0\\ 0&0&3&3 \end{bmatrix} \oplus \begin{bmatrix} 1&0&0&0\\ 0&3&0&0\\ 0&0&2&0\\ 0&0&0&0 \end{bmatrix}.$$

Notice that

$$\Theta = \frac{1}{\sqrt{2}} \begin{bmatrix} 1&-1\\ 1&1 \end{bmatrix}.$$

Therefore, we get by (A.5)

$$L_{\mathbf{e}_1} = \frac{1}{\sqrt{2}} \left(\begin{bmatrix} -2&0&0&0\\ 0&0&0&0\\ 0&0&0&0\\ 0&0&0&-2 \end{bmatrix} \oplus \begin{bmatrix} -1&0&0&0\\ 0&-1&0&0\\ 0&0&-2&0\\ 0&0&0&-2 \end{bmatrix} \oplus \begin{bmatrix} -1&0&0&0\\ 0&-1&0&0\\ 0&0&0&0\\ 0&0&0&0 \end{bmatrix} \right),$$

and

$$L_{\mathbf{e}_2} = \frac{1}{\sqrt{2}} \left(\begin{bmatrix} 4&0&0&0\\ 0&2&0&0\\ 0&0&0&0\\ 0&0&0&2 \end{bmatrix} \oplus \begin{bmatrix} 1&0&0&0\\ 0&1&0&0\\ 0&0&4&0\\ 0&0&0&4 \end{bmatrix} \oplus \begin{bmatrix} 1&0&0&0\\ 0&5&0&0\\ 0&0&4&0\\ 0&0&0&0 \end{bmatrix} \right).$$

Now, we are ready to compute the covariance matrix Σ given in (3.4). Since the mean m is zero and $\rho_\infty = \frac{1}{12}I \oplus \frac{1}{12}I \oplus \frac{1}{12}I$, we are left with

$$\begin{aligned} C_{ij} &= \frac{1}{12} \sum_{e \in A(G_0)} \mathrm{Tr}(B(e)B(e)^*)(\widehat{\theta}(e))_i (\widehat{\theta}(e))_j \\ &\quad + \frac{1}{6} \sum_{e \in A(G_0)} \mathrm{Tr}(B(e)B(e)^* L_{\mathbf{e}_i})(\widehat{\theta}(e))_j \end{aligned}$$

$$=: C_{ij}^{(1)} + C_{ij}^{(2)}. \tag{A.16}$$

For the first term $C_{ij}^{(1)}$, the trace part is all 1 and thus we get

$$C^{(1)} = \frac{1}{3} I.$$

For the second term $C_{ij}^{(2)}$, the terms, before taking trace, are given by

$$\sum_{e \in A(G_0)} (B(e)B(e)^*)(\widehat{\theta}(e))_j$$
$$= \begin{cases} \frac{1}{2\sqrt{2}} \left(\begin{bmatrix} 0 & -2 & 0 & 0 \\ -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \oplus \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \oplus \begin{bmatrix} -2 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \right), & j = 1, \\ \frac{1}{2\sqrt{2}} \left(\begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \oplus \begin{bmatrix} -2 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \oplus \begin{bmatrix} 0 & -2 & 0 & 0 \\ -2 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \right), & j = 2. \end{cases}$$

Then, we get

$$C^{(2)} = \frac{1}{6} \begin{bmatrix} -1 & -1 \\ -1 & 3 \end{bmatrix}.$$

Thus, the covariance matrix is

$$\Sigma = C^{(1)} + C^{(2)} = \frac{1}{6} \begin{bmatrix} 1 & -1 \\ -1 & 5 \end{bmatrix}. \tag{A.17}$$

Notice that the covariance matrix (A.17) has eigenvalues $\frac{1}{6}(3 \pm \sqrt{5})$ with corresponding eigenvectors $[2 \mp \sqrt{5}, 1]^T$.

B Analytic proof of mixture of Gaussians for the hexagonal lattice

Let us recall the Fourier analysis on the crystal lattices and consider a dual process which was developed in [8,9]. For a function $f : \mathbb{L} \to \mathbb{C}$, its Fourier transform $\widehat{f} : \Theta(\mathbb{T}^2) \to \mathbb{C}$ is defined by

$$\widehat{f}(\mathbf{k}) := \sum_{x \in \mathbb{L}} e^{-i\langle \mathbf{k}, x\rangle} f(x), \tag{B.1}$$

and the inverse relation is given by

$$f(x)=\frac{1}{|\det\Theta|}\frac{1}{(2\pi)^2}\int_{\Theta(\mathbb{T}^d)} e^{i\langle \mathbf{k},x\rangle}\widehat{f}(\mathbf{k})d\mathbf{k},\quad x\in\mathbb{L}..$$

(See [8, Section 5.1] for the details.) If $\rho^{(0)}$ is the initial condition, then the state at nth step is given in the Fourier transform space by [7]

$$\widehat{\rho^{(n)}}(\mathbf{k})=\left(\sum_{e\in A(G_0)} e^{-i\langle \mathbf{k},\widehat{\theta}(e)\rangle}L_{B(e)}R_{B(e)^*}\right)^n\widehat{\rho^{(0)}}(\mathbf{k}),\quad \mathbf{k}\in\Theta(\mathbb{T}^2). \tag{B.2}$$

Here, L_A and R_A are the left and right multiplication operators by A, respectively:

$$L_A(B):=AB,\quad R_A(B):=BA.$$

The dual process is the process $(Y_n(\mathbf{k}))_{\mathbf{k}\in\Theta(\mathbb{T}^2)}\in\widehat{\mathcal{A}}$ given by

$$Y_n(\mathbf{k}):=\left(\sum_{e\in A(G_0)} e^{-i\langle \mathbf{k},\widehat{\theta}(e)\rangle}L_{B(e)^*}R_{B(e)}\right)^n(I_{\mathfrak{h}}). \tag{B.3}$$

Then, it holds that

$$p_x^{(n)}=\frac{1}{|\det\Theta|}\frac{1}{(2\pi)^2}\int_{\Theta(\mathbb{T}^2)} e^{i\langle \mathbf{k},x\rangle}\mathrm{Tr}\left(\widehat{\rho^{(0)}}(\mathbf{k})Y_n(\mathbf{k})\right)d\mathbf{k},\quad x\in\mathbb{L}.$$

In other words, the Fourier transform of the probability density $(p_x^{(n)})_{x\in\mathbb{L}}$ at time n is given by

$$\widehat{p_\cdot^{(n)}}(\mathbf{k})=\mathrm{Tr}\left(\widehat{\rho^{(0)}}(\mathbf{k})Y_n(\mathbf{k})\right),\quad \mathbf{k}\in\Theta(\mathbb{T}^2). \tag{B.4}$$

Let us focus on the situation where a mixture of Gaussians appears. Thus, suppose that P_UP_V and P_VP_U are reducible with a common decomposition into communicating classes, say $\{\{1,2\},\{3\}\}$ assuming the stochastic matrices P_UP_V and P_VP_U are defined on the state space $\{1,2,3\}$. Put

$$D(\mathbf{k}):=\mathrm{diag}(e^{-i\langle \mathbf{k},\widehat{\theta}_1\rangle},e^{-i\langle \mathbf{k},\widehat{\theta}_2\rangle},1),$$

where $\mathrm{diag}(a,b,c)$ means the diagonal matrix with entries a, b, and c. We can show (cf. [8, Example 5.3]) that

$$\begin{aligned}&Y_n(\mathbf{k})=A_n(\mathbf{k})\oplus B_n(\mathbf{k});\\&A_n(\mathbf{k})=\mathrm{diag}(a_{n,1}(\mathbf{k}),a_{n,2}(\mathbf{k}),a_{n,3}(\mathbf{k})),\quad B_n(\mathbf{k})=\mathrm{diag}(b_{n,1}(\mathbf{k}),b_{n,2}(\mathbf{k}),b_{n,3}(\mathbf{k})),\end{aligned} \tag{B.5}$$

where the components satisfy the following recurrence relations:

$$\begin{bmatrix} a_{n,1}(\mathbf{k}) \\ a_{n,2}(\mathbf{k}) \\ a_{n,3}(\mathbf{k}) \end{bmatrix} = D(\mathbf{k}) P_U \begin{bmatrix} b_{n-1,1}(\mathbf{k}) \\ b_{n-1,2}(\mathbf{k}) \\ b_{n-1,3}(\mathbf{k}) \end{bmatrix}, \quad \begin{bmatrix} b_{n,1}(\mathbf{k}) \\ b_{n,2}(\mathbf{k}) \\ b_{n,3}(\mathbf{k}) \end{bmatrix} = D(\mathbf{k})^* P_V \begin{bmatrix} a_{n-1,1}(\mathbf{k}) \\ a_{n-1,2}(\mathbf{k}) \\ a_{n-1,3}(\mathbf{k}) \end{bmatrix}. \tag{B.6}$$

Therefore, we get

$$\begin{bmatrix} a_{n,1}(\mathbf{k}) \\ a_{n,2}(\mathbf{k}) \\ a_{n,3}(\mathbf{k}) \end{bmatrix} = \widetilde{A_n}(\mathbf{k}) \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} b_{n,1}(\mathbf{k}) \\ b_{n,2}(\mathbf{k}) \\ b_{n,3}(\mathbf{k}) \end{bmatrix} = \widetilde{B_n}(\mathbf{k}) \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}. \tag{B.7}$$

Here, the matrices $\widetilde{A}_n(\mathbf{k})$ and $\widetilde{B}_n(\mathbf{k})$ are given by

$$\widetilde{A}_n(\mathbf{k}) = \begin{cases} (D(\mathbf{k}) P_U D(\mathbf{k})^* P_V)^m, & n = 2m, \\ (D(\mathbf{k}) P_U D(\mathbf{k})^* P_V)^m D(\mathbf{k}) P_U, & n = 2m+1, \end{cases} \tag{B.8}$$

$$\widetilde{B}_n(\mathbf{k}) = \begin{cases} (D(\mathbf{k})^* P_V D(\mathbf{k}) P_U)^m, & n = 2m, \\ (D(\mathbf{k})^* P_V D(\mathbf{k}) P_U)^m D(\mathbf{k})^* P_V, & n = 2m+1. \end{cases} \tag{B.9}$$

By the assumption, we see that the operators $\widetilde{A}_n(\mathbf{k})$ and $\widetilde{B}_n(\mathbf{k})$ are block diagonal matrices acting on $\mathbb{C}^2 \oplus \mathbb{C}$. And since it is irreducible for each block, when we restrict on each block, the map $\mathcal{L}_*$ has a unique invariant state (see the proof of [8, Proposition 4.1]). Therefore, for any $\lambda \in [0, 1]$, the following states (density matrices) are all invariant states satisfying $\mathcal{L}_*(\rho^{(\lambda)}) = 0$:

$$\rho^{(\lambda)} = \lambda\eta + (1-\lambda)\xi, \quad \eta = \frac{1}{2}\eta_0 \oplus \frac{1}{2}\eta_0, \quad \xi = \frac{1}{2}\xi_0 \oplus \frac{1}{2}\xi_0 \tag{B.10}$$

with

$$\eta_0 := \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \xi_0 := \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

For a concrete model, let us consider $U = V = U_H$ in (4.12). By (4.14), $P_U P_V$ and $P_V P_U$ are reducible with a common communicating classes. There are infinitely many solutions to the equation $\mathcal{L}_*(\rho) = 0$, and in fact, for any $\lambda \in [0, 1]$, the states $\rho^{(\lambda)}$ in (B.10) are all invariant states.

A Gaussian Let us take the initial state

$$\rho^{(0)} = \rho_1^{(0)} := \left(\frac{1}{2}\eta_0 \oplus \frac{1}{2}\eta_0\right) \otimes |0\rangle\langle 0|. \tag{B.11}$$

Hence, we have $\widehat{\rho^{(0)}}(\mathbf{k}) = \frac{1}{2}\eta_0 \oplus \frac{1}{2}\eta_0$. Therefore, putting $u := [1, 1, 1]^T$ and $u_0 := \frac{1}{\sqrt{2}}[1, 1, 0]^T$ we see that (use also $\widetilde{B}_n(\mathbf{k}) = \overline{\widetilde{A}_n(\mathbf{k})}$)

$$\widehat{p^{(n)}_{\cdot}}(\mathbf{k}) = \mathrm{Tr}\left(\widehat{\rho^{(0)}}(\mathbf{k}) Y_n(\mathbf{k})\right) = \mathrm{Re}\langle u_0, \widetilde{A}_n(\mathbf{k}) u_0\rangle.$$

Putting $\theta_j = -\langle \mathbf{k}, \widehat{\theta}_j\rangle$, $j = 1, 2$, for simplicity, we have $D = \mathrm{diag}(e^{i\theta_1}, e^{i\theta_2}, 1)$. By defining $P_\pm := D^{\pm 1/2} P D^{\mp 1/2}$, we can write

$$\widetilde{A}_n = \begin{cases} D^{1/2}(P_+P_-)^m D^{1/2}, & n = 2m+1, \\ D^{1/2}(P_+P_-)^{m-1} P_+ D^{-1/2}, & n = 2m. \end{cases}$$

(We have used $Pu = u$.) Consider firstly $n = 2m+1$. Putting $u_\pm := D^{\pm 1/2} u_0$, we have

$$\widehat{p^{(n)}_{\cdot}}(\mathbf{k}) = \mathrm{Re}\langle u_-, (P_+P_-)^m u_+\rangle, \quad (n = 2m+1)$$

We notice that D and P, and hence $P^\pm$ also, are invariant on the range of $P_1^\perp$, i.e., the two-dimensional subspace generated by the first two components of the vectors in $\mathbb{C}^3$. Therefore, without loss of generality, we may let

$$u_0 := \frac{1}{\sqrt{2}}[1, 1]^T, \quad D := \mathrm{diag}(e^{i\theta_1}, e^{i\theta_2}), \quad P = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}.$$

We notice that

$$P_\pm = |u_\pm\rangle\langle u_\pm|.$$

By directly computing, we get

$$\begin{aligned}(P_+P_-)|u_+\rangle &= \mu^2 |u_+\rangle \\ (P_+P_-)|u_-\rangle &= \langle u_+, u_-\rangle |u_+\rangle.\end{aligned}$$

Here,

$$\mu := |\langle u_+, u_-\rangle| = \frac{1}{2}\left|e^{i\theta_1} + e^{i\theta_2}\right|.$$

Therefore,

$$\widehat{p^{(n)}_{\cdot}}(\mathbf{k}) = \mathrm{Re}\langle u_-, (P_+P_-)^m u_+\rangle = \mu^{2m}\mathrm{Re}\langle u_-, u_+\rangle = \frac{1}{2}(\cos\theta_1 + \cos\theta_2)\mu^{2m}.$$

Now, let us consider the asymptotics of $\widehat{p^{(n)}_{\cdot}}(\mathbf{k})$ for large n. Let $X_n \in \mathbb{L}$ be the position of the walker at time n. We want to see the behavior of $X_n/\sqrt{n}$ at large time by computing $\mathbb{E}\left[e^{i\langle \mathbf{t}, X_n/\sqrt{n}\rangle}\right]$, which is nothing but $\widehat{p_{\cdot}^{(n)}}(-\mathbf{t}/\sqrt{n})$ by (B.1). Then, formerly defined $\theta_j = -\langle \mathbf{k}, \widehat{\theta}_j\rangle$ becomes now $\theta_j = \frac{1}{\sqrt{n}}\langle \mathbf{t}, \widehat{\theta}_j\rangle$, $j = 1, 2$, and we get

$$\frac{1}{2}(\cos\theta_1 + \cos\theta_2) = 1 + O\left(\frac{1}{n}\right),$$
$$\mu^2 = \frac{1}{2}\left(1 + \cos(\theta_1 - \theta_2)\right) = 1 - \frac{\varepsilon^2(\mathbf{t})}{4n} + O\left(\frac{1}{n^2}\right),$$

where $\varepsilon^2(\mathbf{t}) = \langle \mathbf{t}, \widehat{\theta}_1 - \widehat{\theta}_2\rangle^2$. Therefore, as $n \to \infty$,

$$\mathbb{E}\left[e^{i\langle \mathbf{t}, X_n/\sqrt{n}\rangle}\right] = \widehat{p_{\cdot}^{(n)}}(-\mathbf{t}/\sqrt{n}) \to e^{-\frac{1}{8}\varepsilon^2(\mathbf{t})} = e^{-\frac{1}{4}t_1^2}.$$

We conclude that $X_n/\sqrt{n}$ converges weakly to a Gaussian with covariance

$$\Sigma = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{B.12}$$

The limit as n goes to infinity with even numbers can be computed similarly, and it gives the same result as the above. It is easy to guess the above result from the dynamics of the walk. In fact, the movements in the y-direction are just an oscillation between the coordinates $\{-1/\sqrt{2}, 0, 1/\sqrt{2}\}$. Therefore, the variance in the y-direction of the scaled walk by $1/\sqrt{n}$ converges to 0 as (B.12) shows.

Another Gaussian Let us take the initial state

$$\rho^{(0)} = \rho_2^{(0)} := \left(\frac{1}{2}\xi_0 \oplus \frac{1}{2}\xi_0\right) \otimes |0\rangle\langle 0|. \tag{B.13}$$

Put $v_0 := [0, 0, 1]^T$ and P_2 which is the projection onto the third component space so that $v_0 = P_2 u$. Now, we have $\widehat{\rho^{(0)}}(\mathbf{k}) = \frac{1}{2}\xi_0 \oplus \frac{1}{2}\xi_0$. Therefore,

$$\widehat{p_{\cdot}^{(n)}}(\mathbf{k}) = \mathrm{Tr}\left(\widehat{\rho^{(0)}}(\mathbf{k}) Y_n(\mathbf{k})\right) = \mathrm{Re}\langle v_0, \widetilde{A}_n(\mathbf{k}) v_0\rangle.$$

Here, we have used again the fact that $\widetilde{B}_n(\mathbf{k}) = \overline{\widetilde{A}_n(\mathbf{k})}$. Clearly, we have

$$\widehat{p_{\cdot}^{(n)}}(\mathbf{k}) = 1.$$

This means that the measure is a Dirac measure at the origin. From the dynamics of the walk, it is obvious why we have Dirac measure. In fact, from the initial condition, the walk never moves out of the origin.

A mixture of Gaussians Let us consider an initial condition given by a convex combination of the preceding examples:

$$\rho_\lambda^{(0)} := \lambda\rho_1^{(0)} + (1 - \lambda)\rho_2^{(0)},$$

where $\rho_1^{(0)}$ and $\rho_2^{(0)}$ are in (B.11) and (B.13), respectively. As we have seen in the preceding examples, the states $\rho_1^{(0)}$ and $\rho_2^{(0)}$ never mix as the dynamics goes on. Therefore, we see that as $n \to \infty$, $X_n/\sqrt{n}$ converges weakly to the mixture of Gaussians

$$\lambda\mu^{(1)} + (1-\lambda)\delta_0,$$

where $\mu^{(1)}$ is a Gaussian with mean 0 and covariance Σ in (B.12).

References

1. Attal, S., Guillotin-Plantard, N., Sabot, C.: Central limit theorems for open quantum random walks and quantum measurement records. Ann. Henri Poincaré **16**(1), 15–43 (2015)
2. Attal, S., Petruccione, F., Sabot, C., Sinayskiy, I.: Open quantum random walks. J. Stat. Phys. **147**, 832–852 (2012)
3. Attal, S., Petruccione, F., Sinayskiy, I.: Open quantum walks on graphs. Phys. Lett. A **376**(18), 1545–1548 (2012)
4. Fagnola, F., Rebolledo, R.: Transience and recurrence of quantum Markov semigroups. Probab. Theory Relat. Fields **126**, 289–306 (2003)
5. Fagnola, F., Rebolledo, R.: Quantum Markov semigroups and their stationary states, Stochastic analysis and mathematical physics II. Trends Math. pp. 77–128, (2003)
6. Fagnola, F., Pellicer, R.: Irreducible and periodic positive maps. COSA **3**(3), 407–418 (2009)
7. Ko, C.K., Konno, N., Segawa, E., Yoo, H.J.: How does Grover walk recognize the shape of crystal lattice? Quantum Inf. Process. **17**(7), 167 (2018)
8. Ko, C.K., Konno, N., Segawa, E., Yoo, H.J.: Central limit theorems for open quantum random walks on the crystal lattices. J. Stat. Phys. **176**, 710–735 (2019)
9. Konno, N., Yoo, H.J.: Limit theorems for open quantum random walks. J. Stat. Phys. **150**, 299–319 (2013)
10. Sunada, T.: Topological crystallography with a view towards discrete geometric analysis, Surveys and Tutorials in Applied Mathematical Sciences 6. Springer (2013)
11. Umanita, V.: Classification and decomposition of quantum Markov semigroups. Thesis, Politecnico di Milano (2005)
12. Umanita, V.: Classification and decomposition of quantum Markov semigroups. Probab. Theory Relat. Fields **134**, 603–623 (2006)