Spectral and asymptotic properties of Grover walks on crystal lattices

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Abstract. We propose twisted Szegedy walk to estimate limit behavior of a discrete-time quantum walk on infinite abelian covering graphs. Firstly, we show that the spectrum of the twisted Szegedy walk on the quotient graph is expressed by mapping the spectrum of a twisted random walk to the unit circle. Secondly, we find that the spatial Fourier transform of the twisted Szegedy walk with some appropriate parameters becomes the Grover walk on its infinite abelian covering graph. Finally, as this application, we show that if the Betti number of the quotient graph is strictly greater than one, then localization is ensured with some appropriated initial state. Moreover the limit density function for the Grover walk on \( \mathbb{Z}^d \) with flip flop shift, which implies the coexistence of linear spreading and localization, is computed. We partially obtain its abstractive shape; the support of the density is within the \( d \)-dimensional sphere whose radius is \( 1/\sqrt{d} \), and there are \( 2^d \) singular points on the surface of the sphere.

1 Introduction

Quantum walks are intensively studied from the various kinds of view points, whose primitive form, discrete-time quantum walk on \( \mathbb{Z} \), can be seen in so called Feynman’s checker board [3]. A discrete-time quantum walk itself was presented in the study of the quantum probabilistic theory proposed by [4]. The Grover walk on general graph has been appeared in [20]. This walk is one of the most intensively-investigated quantum walks from the view point of a quantum information theory and a spectral graph theory [1, 5], which accomplishes quantum

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speed up search algorithms in some cases. A review around here can be seen in [1]. The Szegedy walk, which is a generalization of the Grover walk, was proposed to provide more abstractive discussion to these search algorithms [17](2004). One of the advanced points of the Szegedy walk is that the spectrum is decomposed into two sets: the arccosine of the spectrum for an underlying reversible random walk and \{±1\} with some multiplicities. As its application of the spectrum theory, the performance of the quantum search algorithm based on the Szegedy walk is usually evaluated by hitting time of the random walk behind the Szegedy walk.

In this paper, we introduce “twisted” Szegedy walk acting on \(\ell^2(D)\) for a given graph \(G = (V, D)\), where \(V\) and \(D\) are the set of vertices and arcs, respectively. In parallel, we also present a twisted (random) walk on \(\ell^2(V)\) behind the quantum walk on \(\ell^2(D)\) for the purpose of providing the mapping theory as is the original Szegedy walk. Study on this twisted random walk has been well developed; for example some effects of the spatial structure of the crystal lattice on the return probability and central limit theorems of the random walk are found in [11, 12]. To see the relationship between the spectra of the twisted random walk and the twisted Szegedy walk, we introduce new boundary operators \(d_A, d_B : \ell^2(D) \rightarrow \ell^2(V)\). Then we show \(L \equiv \mathbb{C}d_A^*(\ell^2(V)) + \mathbb{C}d_B^*(\ell^2(V)) \subseteq \ell^2(D)\) is invariant under the action of the twisted Szegedy walk. Here \(d_A, d_B : \ell^2(V) \rightarrow \ell^2(D)\) are the adjoint operators of \(d_A\) and \(d_B\), respectively. Observing carefully the above, we find that the eigenvalues of the twisted random walk on \(\ell^2(V)\) describe the “real parts” of eigenvalues of the quantum walk (Proposition 1). Thus we call the eigenspace \(L\) inherited part from the twisted random walk. On the other hand, the rest of the eigenspace; \(L^\perp\), is expressed by the intersection of the kernels of the boundary operators \(d_A\) and \(d_B\). As \(\ker(\partial)\) is generated by all the closed paths of \(G\) for a usual boundary operator of graphs \(\partial : C_1 \rightarrow C_0\), the orthogonal complement space \(L^\perp = \ker(d_A) \cap \ker(d_B)\) is also characterized by all the closed paths of \(G\) (Theorem 1). Here \(C_1 = \sum_{e \in E(G)} \mathbb{Z}\delta_e\) and \(C_0 = \sum_{v \in V(G)} \mathbb{Z}\delta_v\). This fact implies that there is a homological abstraction within the Grover walk and plays important role to provide a typical stochastic behavior called localization which can be seen in Theorem 2.

There are many kinds of the mapping theorems. For example, in [7], it is discussed how the spectra of the Laplacian changes under graph-operations; that is, spectral mapping theorems from the spectrum of the Laplacian of the original graph \(G\) to ones of line graph \(LG\) and subdivision graph \(SG\) and para-line graph \(PG\) of the original graph \(G\), respectively. Our work stands for another kind of mapping theorem to discrete-time quantum walk in this sense. On the other hand, we use the vector potential, which corresponds to our twist here, in the context of the quantum graph in [6]. We have partially succeeded in finding a spectral mapping theorem and a relationship between a discrete-time quantum walk and the quantum graph of a finite regular covering graph. A spectral result on quantum walks on a graph with two infinite half lines is also obtained in [2] from the view point of a scattering quantum theory. Analyzing the connection between them more clearly is one of the interesting future’s problems.

As an effective application of this mapping theorem, we show the specific stochastic properties named localization and linear spreading in the Grover walk on crystal lattice in some cases. We find that the localization is due to the existence of cycles in the crystal lattice. More precisely, if the Betti number of the quotient graph is strictly greater than 1, then the localization is ensured with the overlap between some appropriate initial state and a
obtained. For example, in the case of special quantum coins [19] for example, its limit distribution is explicitly obtained. For d ≥ 3 case, although the return probability at the origin with moving shift is discussed in [15], almost all the behaviors for d ≥ 3 case have not been clarified yet up to now. Here we partially obtain the shape of the limit distribution on Z^d for the Grover walk: we show that the support of the density function is contained by d-dimensional ball whose radius is 1/√d and 2^d singular points exist on the surface of the d-dimensional ball (Theorems 5 and 6).

This paper is organized as follows. In Sect. 2, we propose the twisted Szegedy walk and provide the mapping theory of the spectrum of the twisted Szegedy walk from a twisted walk. We devote to the Grover walk on crystal lattice and its Fourier transform in Sect. 3. The linear spreading and localization are shown. Finally we compute the limit density function of the Grover walk on Z^d in Sect. 4.

2 Twisted Szegedy walks on finite graphs

At first we explain our setting of graph. Let G = (V(G), E(G)) be a connected graph (having possibly multiple edges and self-loops) with the set V = V(G) of vertices and the set E = E(G) of unoriented edges. We naturally introduce the set of arcs D(G) from E(G) as follows; For an arc e ∈ D(G), the origin vertex and the terminal one of e are denoted by o(e) and t(e), respectively. The inverse arc of e is denoted by ¯e. So e ∈ D iff o(e)t(e) ∈ E(G). For a vertex v of G, deg(v) stands for degree of v. A path p is a sequence of arcs (e_1, e_2, ..., e_n) with t(e_j) = o(e_{j+1}) for any j ∈ {1, ..., n}. We denote the origin and terminus of path p as o(p), and t(p), respectively. If {o(e_j)}_{j=1}^n are distinct, then the path p is called a simple path. We define the set of all paths and simple ones of graph G by P(G) and P_0(G). If t(e_n) = o(e_1) for p = (e_1, e_2, ..., e_n) ∈ P_0(G) holds, then p is called essential cycle.

We denote the standard basis of ℓ^2(D(G)) as δ_e, (e ∈ D(G)), such that δ_e(f) = 1, (e = f), = 0, (e ≠ f). At each vertex u ∈ V(G), we define subspace ℋ_u ⊂ ℓ^2(D(G)) by

ℋ_u = span{δ_e; o(e) = u}.

Thus ℓ^2(D(G)) = ⊕_{u∈V(G)} ℋ_u is hold. Define w : D(G) → C called weight such that w(e) ≠ 0 for all e ∈ D(G) and

\[ \sum_{e:o(e)=u} |w(e)|^2 = 1 \text{ for all } u \in V(G). \]

Put θ : D(G) → R called 1-form satisfying

\[ \theta(\bar{e}) = -\theta(e) \text{ for any } e \in D(G). \]
Remark 1. The coin operator \( \ell \) boundary operators: let \( d_A, d_B : \ell^2(D(G)) \to \ell^2(V(G)) \) be for \( \phi \in \ell^2(D(G)) \) and \( v \in V(G) \),

\[
(d_A \phi)(v) = \sum_{e:o(e)=v} \phi(e)w(e), \quad (d_B \phi)(v) = \sum_{e:o(e)=v} \phi(\bar{e})w(e)e^{-i\theta(e)}
\]

(2.1)

respectively. The coboundary operators of \( d_A^* \) and \( d_B^* \) are determined by for \( f \in \ell^2(V(G)) \) and \( e \in D(G) \),

\[
(d_A^* f)(e) = w(e)f(o(e)), \quad (d_B^* f)(e) = e^{-i\theta(e)}w(\bar{e})f(t(e)),
\]

(2.2)

respectively from the relationship \( \langle \phi, d_J^* f \rangle_D = \langle d_J \phi, f \rangle_V \) \( (J \in \{A, B\}) \) with \( f \in \ell^2(V(G)) \), \( \phi \in \ell^2(D(G)) \). Here for any \( \phi_1, \phi_2 \in \ell^2(D(G)) \) and \( f_1, f_2 \in \ell^2(V(G)) \),

\[
\langle \phi_1, \phi_2 \rangle_D = \sum_{e \in D(G)} \phi_1(e)\phi_2(e), \quad \langle f_1, f_2 \rangle_V = \sum_{v \in V(G)} f_1(v)f_2(v).
\]

The twisted Szegedy walk associated with the weight \( w \) and 1-form \( \theta \) treated here is defined as follows:

1. The total state space \( \mathcal{H} : \mathcal{H} = \ell^2(D) \).

2. Time evolution \( U^{(w, \theta)} : U^{(w, \theta)} = S^{(\theta)} C^{(w)} \). Here
   
   (a) Coin operator: \( C^{(w)} = 2d_A^*d_A - I \)
   
   (b) (twisted) Shift operator: for \( f \in \ell^2(D(G)) \), \( (S^{(\theta)} f)(e) = e^{-i\theta(e)}f(\bar{e}) \).

**Remark 1.** The coin operator \( C^{(w)} \) can be decomposed into \( |V| \)-unitary operators such that \( C^{(w)} = \bigoplus_{u \in V} H^{(u)} \), where \( H^{(u)} : \mathcal{H}_u \to \mathcal{H}_u \) is the following unitary operator on \( \mathcal{H}_u \)

\[
\langle \delta f, H^{(u)} \delta e \rangle = \mathbf{1}_{o(e)=o(f)=u} \left( 2w(e)w(f) - \delta_{e,f} \right).
\]

\( H^{(u)} \) is called local quantum coin of \( C^{(w)} \) assigned at vertex \( u \).

For each \( e \in D(G) \), we introduce \( P(e) : \mathcal{H}_{o(e)} \to \mathcal{H}_{t(e)} \) by

\[
P(e) = \Pi_{\delta_e} U^{(w, \theta)} \Pi_{\mathcal{H}_{o(e)}}.
\]

Here for subset \( \mathcal{H}' \subset \mathcal{H} \), \( \Pi_{\mathcal{H}'} \) is the orthogonal projection onto \( \mathcal{H}' \). Given an initial state \( \Psi_0 \in \ell^2(D(G)) \) with \( ||\Psi_0||^2 = 1 \), let \( \Psi_n : V(G) \to \ell^2(D(G)) \) be \( \Psi_n(u) = \Pi_{\mathcal{H}_u}(U^{(w, \theta)})^n \Psi_0 \) for \( n \in \mathbb{N} \). Then we have the following recurrence relation:

\[
\Psi_n(u) = \sum_{e:t(e)=u} P(e)\Psi_{n-1}(o(e)), \quad (n \geq 1),
\]

since

\[
\Psi_n(u) = \Pi_{\mathcal{H}_u}(U^{(w, \theta)}) \sum_{v \in V(G)} \Psi_{n-1}(v) = \sum_{e:o(e)=u} \Pi_{\delta_e}(U^{(w, \theta)})\Psi_{n-1}(o(\bar{e}))
\]

\[
= \sum_{e:o(e)=u} \Pi_{\delta_e}(U^{(w, \theta)})\Pi_{\mathcal{H}_u} \Psi_{n-1}(o(\bar{e})) = \sum_{e:t(e)=u} P(e)\Psi_{n-1}(o(e)).
\]
This is an analogous expression to random walk \( \{ p(e) : e \in D(G) \} \) with \( p(e) \in (0, 1) \) and \( \sum_{e: \ell(e) = u} p(e) = 1 \), on the other hand, \( \{ P(e) : e \in D(G) \} \) with \( P(e) : \mathcal{H}_{\ell(e)} \rightarrow \mathcal{H}_{\ell(e)} \) and \( \sum_{e: \ell(e) = u} P(e) = H^{(u)} \in \text{SU}(\text{deg}(u)) \). The unitarity of the time evolution provides the sequence of distribution \( \{ \mu_n \}_n \) such that \( \mu_n : V(G) \rightarrow [0, 1] \) with \( \mu_n(u) = ||\Psi_n(u)||^2 \). We denote a random variable \( X_n \) following \( \mu_n \). Our interest is a sequence of random variables \( \{ X_n \}_n \) induced by the twisted Szegedy walk as is seen in the last half of this paper.

**Remark 2.** Define \( D^{(\theta)} : \ell^2(D(G)) \rightarrow \ell^2(D(G)) \) such that \( D^{(\theta)}f(e) = e^{i\theta(e)}f(e) \). This generalized Szegedy walk can be rewritten by \( U^{(w, \theta)} = S^{(0)}C^{(w, \theta)}, \) where \( C^{(w, \theta)} = D^{(\theta)}C \) and \( S^{(0)} \) is the usual flip flop shift operator; that is, \( S^{(\theta)} \) with \( \theta(e) = 0 \) for every \( e \in D \). Thus the local quantum coin assigned at \( u \) is described by

\[
\langle \delta_f, \tilde{H}^{(u)}\delta_e \rangle = e^{i\theta(f)}\langle \delta_f, H^{(u)}\delta_e \rangle
\]

By the way, on some regular graphs, there may exist two possible choices of the shift operators; moving shift \( S_m \) and flip flop shift \( S_f \). For example, in \( \mathbb{Z} \) case,

\[
(S_m\psi)((x, x + j)) = \psi((x - j, x)), \quad (S_f\psi)((x, x + j)) = \psi((x + j, x)), \quad (j \in \{ \pm 1 \}, x \in \mathbb{Z}).
\]

The moving shift keeps the direction of arcs while the flip flop shift reverses the directions. However on general graph, the direction is not determined uniquely and so is moving shift operator. Moreover, taking a permutation to each local coin operator of the flip flop shift type quantum walk provides any moving shift type quantum walks. For example, for \( \mathbb{Z} \) case, the following relationship between the time evolution of flip flop shift \( U_f(H) \) and moving shift \( U_m(H) \) with local coin operator \( H \) holds;

\[
U_m(H) = \mathcal{P}U_f(HP)\mathcal{P}.
\]

Here \( \mathcal{P}g((x, x+j)) = g((x, x-j)) \). See Sect. 2 in [5] for more detailed and general discussions. From these reasons, we apply the flip flop shift operator in this paper. Discrete-time quantum walks on several graphs with moving shift can be seen, for example triangular lattice in [10, 18].

**Remark 3.** It is hold that \( d_Ad_A^* = d_Bd_B^* = I_V \). On the other hand, the operations \( d_A^*d_A \) and \( d_B^*d_B \) are the projections onto the subspaces

\[
\mathcal{A} \equiv d_A^*(\ell^2(V)) \subset \ell^2(D) \quad \text{and} \quad \mathcal{B} \equiv d_B^*(\ell^2(V)) \subset \ell^2(D),
\]

respectively. So we have

\[
d_A(\ell^2(D)) = d_B(\ell^2(D)) = \ell^2(V).
\]

We prepare an important Hermite operator given by a pair of \( w \) and \( \theta \), \( T^{(w, \theta)} : \ell^2(V) \rightarrow \ell^2(V) \) such that \( T^{(w, \theta)} = d_A d_B^* \). We call \( T^{(w, \theta)} \) discriminant operator of \( U^{(w, \theta)} \). Applying Eqs. (2.2) and (2.1), we have for \( u, v \in \ell^2(V), \)

\[
\langle \delta_v, T^{(w, \theta)}\delta_u \rangle = \sum_{f: \omega(f) = u, \tau(f) = v} w(f)\overline{w(f)} e^{i\theta(f)}. \tag{2.4}
\]
On the other hand, from the definition of $T^{(w,\theta)}$ and Remark 3, we have another expression for $T^{(w,\theta)}$:

$$T^{(w,\theta)} = d_A \Pi_A S^{(\theta)} \Pi_A d_A^*.$$  \hspace{1cm} (2.5)

**Proposition 1.**

(1) **Eigenvalues:** Denote $m_{\pm 1}$ by the multiplicities of the eigenvalues for $T^{(w,\theta)}$, respectively. Let $\varphi_{QW} : \mathbb{R} \to \mathbb{R}$ such that $\varphi_{QW}(x) = (x + x^{-1})/2$. Then we have

$$\text{spec}(U^{(w,\theta)}) = \varphi_{QW}^{-1}\left(\text{spec}(T^{(w,\theta)})\right) \cup \{1\}^M \cup \{-1\}^M,$$  \hspace{1cm} (2.6)

where $M = \max\{0, |E| - |V| + m_1\}$, $M = \max\{0, |E| - |V| + m_{-1}\}$.

(2) **Eigenspace:** The eigenspace of eigenvalues $\varphi_{QW}^{-1}\left(\text{spec}(T^{(w,\theta)})\right)$, $\mathcal{L}$, is

$$\mathcal{L} = \mathbb{C}d_A^*(\ell^2(V)) + \mathbb{C}d_B^*(\ell^2(V)).$$

The normalized eigenvector for the eigenvalue $e^{i\phi} \in \varphi_{QW}^{-1}\left(\text{spec}(T^{(w,\theta)})\right)$ is expressed by

$$\frac{1}{\sqrt{2}} \frac{1}{\sin \phi} \left(1 + (\sqrt{2} - 1)1_{\{\phi \in \{0, \pi\}\}}\right) (I - e^{i\phi} S^{(\theta)}) d_A^* \nu_{\phi},$$

where $\nu_{\phi} = \nu_{-\phi} \in \ell^2(V)$ is the eigenfunction of $T^{(w,\theta)}$ of eigenvalue $\cos \phi$ with $||\nu|| = 1$. On the other hand, its orthogonal complement space is expressed by

$$\mathcal{L}^\perp = \ker(d_A) \cap \ker(d_B).$$

The eigenspaces corresponding to eigenvalues $\{1\}^M$ and $\{-1\}^M$ are described by

$$\ker(d_A) \cap \mathcal{H}^{(S)}_\pm \quad \text{and} \quad \ker(d_B) \cap \mathcal{H}^{(S)}_\pm,$$  \hspace{1cm} (2.7)

respectively. Here

$$\mathcal{H}^{(S)}_\pm = \text{span}\{\delta_f \pm e^{i\theta(f)} \delta_f; f \in D(G)\},$$

in other words $\mathcal{H}^{(S)}_\pm$ are the eigenspaces of $S^{(\theta)}$ whose eigenspace are $\pm 1$, respectively.

**Proof.** At first, we show that the absolute value of eigenvalue of $T^{(w,\theta)}$ is bounded as follows: when $T^{(w,\theta)}g = \lambda g$ for $g \in \ell^2(V)$, $\lambda \in \mathbb{R}$ because $T^{(w,\theta)}$ is an Hermite operator. Moreover we have from Eq. (2.5),

$$||| \lambda ||^2 ||g||^2 = ||T^{(w,\theta)}g||^2 = ||\Pi_A S^{(\theta)} \Pi_A \psi ||^2 \leq ||S^{(\theta)} \Pi_A \psi ||^2 = ||\Pi_A \psi ||^2 \leq ||\psi||^2 = ||g||^2,$$  \hspace{1cm} (2.8)

where $\psi = d_A^* g \in \ell^2(D)$. By Eq. (2.5), the second equation derives from $||T^{(w,\theta)}g||^2 = \langle d_A^* \psi, T^{(w,\theta)} d_A^* \psi \rangle = \langle \psi, d_A T^{(w,\theta)} d_A^* \psi \rangle = \langle \psi, S^{(\theta)} \Pi_A \psi \rangle$. Remark 3 implies $||\psi||^2 = (d_A^* g, d_A^* g) = \langle g, d_A d_A^* g \rangle = ||g||^2$. Thus all the eigenvalues of $T^{(w,\theta)}$ lives in $[-1, 1]$. By the way, noting $C^{(w)} d_A^* = d_A^*$ and $C^{(w)} d_B^* = 2 d_A^* T^{(w,\theta)} - d_B^*$ implies that

$$U^{(\theta, w)} d_A^* = d_B^*, \quad U^{(\theta, w)} d_B^* = 2 d_A^* T^{(w,\theta)} - d_A^*.$$  \hspace{1cm} (2.9)

$$U^{(\theta, w)} d_B^* = 2 d_B^* T^{(w,\theta)} - d_B^*.$$  \hspace{1cm} (2.10)
When we choose $\nu_\phi \in l^2(V)$ as the eigenfunction of $T^{(w,\theta)}$ of eigenvalue $\cos \phi$, we can observe that $\text{span}\{d^*_A \nu_\phi, d^*_B \nu_\phi\} \subset \mathcal{L}$ are invariant under the action $U^{(w,\theta)}$ as follows:

\[
U^{(\theta,w)} \rho_\phi = S^{(\theta)} \rho_\phi, \quad (2.11)
\]
\[
U^{(\theta,w)} S^{(\theta)} \rho_\phi = 2 \lambda S^{(\theta)} \rho_\phi - \rho_\phi, \quad (2.12)
\]

where $\rho_\phi = d^*_A \nu_\phi$. Define $\mathcal{L}_\lambda \equiv \text{span}\{\rho_\phi, S^{(\theta)} \rho_\phi\}$, where $\lambda = \cos \phi$. It is hold that

\[
\mathcal{L} = \bigoplus_{\lambda \in \text{spec}(T^{(w,\theta)})} \mathcal{L}_\lambda. \quad (2.13)
\]

Since

\[
|\langle \rho_\phi, S^{(\theta)} \rho_\phi \rangle| = |\langle d^*_A \nu_\phi, S^{(\theta)} d^*_A \nu_\phi \rangle| = |\langle \nu_\phi, d_A S^{(\theta)} d^*_A \nu_\phi \rangle| = |\langle \nu_\phi, T^{(w,\theta)} \nu_\phi \rangle| = \cos \phi,
\]

the value $\phi \in \mathbb{R}$ is so called geometric angle between $\rho_\phi$ and $S^{(\theta)} \rho_\phi$. Thus if $\phi \in \{n\pi; n \in \mathbb{N}\}$, then $\rho_\phi$ and $S^{(\theta)} \rho_\phi$ are linearly dependent, otherwise, linearly independent.

(1) $\phi \in \{n\pi; n \in \mathbb{N}\}$ case: Since in this case, $\langle \rho_\phi, S^{(\theta)} \rho_\phi \rangle \in \{\pm 1\}$, $S^{(\theta)} \rho_0 = \rho_0$ and $S^{(\theta)} \rho_\pi = -\rho_\pi$ hold. So we have

\[
\mathcal{L}_1 \subset \mathcal{H}_+^{(S)} \text{ and } \mathcal{L}_{-1} \subset \mathcal{H}_-^{(S)}. \quad (2.14)
\]

From Eq. (2.11),

\[
U^{(w,\theta)} \rho_0 = \rho_0 \quad \text{and} \quad U^{(w,\theta)} \rho_\pi = -\rho_\pi. \quad (2.15)
\]

(2) $\phi \notin \{n\pi; n \in \mathbb{N}\}$ case: In the subspace $\mathcal{L}_{\cos \phi} = \text{span}\{\rho_\phi, S^{(\theta)} \rho_\phi\}$,

\[
U^{(w,\theta)} \approx \begin{bmatrix}
0 & -1 \\
1 & 2 \cos \phi
\end{bmatrix},
\]

where $\rho_\phi \approx T[1,0]$ and $S^{(\theta)} \rho_\phi \approx T[0,1]$. Then the eigenvalues and its normalized eigenvectors of eigenspace $\mathcal{L}_{\cos \phi}$ are expressed by

\[
e^{\pm i\phi}, \text{ and } \omega_{\pm \phi} = \frac{1}{\sqrt{2|\sin \phi|}}(I - e^{\pm i\phi} S^{(\theta)}) \rho_{\pm \phi}, \quad (2.16)
\]

respectively. By the way, we can observe that

\[
S^{(\theta)} \omega_\phi = -e^{i\phi} \omega_{-\phi}, \quad S^{(\theta)} \omega_{-\phi} = -e^{-i\phi} \omega_\phi,
\]

which implies

\[
\omega_\phi + e^{i\phi} \omega_{-\phi} \in \mathcal{H}_-^{(S)}, \quad \omega_{-\phi} - e^{i\phi} \omega_{-\phi} \in \mathcal{H}_+^{(S)}
\]

So we have

\[
\dim(\mathcal{L}_{\cos \phi} \cap \mathcal{H}_+^{(S)}) = \dim(\mathcal{L}_{\cos \phi} \cap \mathcal{H}_-^{(S)}) = 1 \quad (2.17)
\]
Combining Eqs. (2.14) and (2.17), we have
\[ \dim(\mathcal{H}_+^{(S)} \cap \mathcal{L}) = |V| - m_{-1} \quad \text{and} \quad \dim(\mathcal{H}_-^{(S)} \cap \mathcal{L}) = |V| - m_1. \] (2.18)

On the other hand, from now on we consider the orthogonal complement space of \( \mathcal{L} \). From a direct computation, we have \( \psi \in \mathcal{H}_-^{(S)} \) and \( \phi \in \mathcal{H}_+^{(S)} \) iff
\[ \psi(e) = -e^{-i\theta(e)} \psi(\bar{e}), \] (2.19)
\[ \phi(e) = e^{-i\theta(e)} \phi(\bar{e}), \] (2.20)
respectively. For any \( \psi \in \mathcal{L}^\perp \), it is hold that
\[ \psi \xmapsto{C^{(w)}} -\psi \xmapsto{S^{(w)}} -S^{(\theta)} \psi, \] (2.21)
\[ S^{(\theta)} \psi \xmapsto{C^{(w)}} -S^{(\theta)} \psi \xmapsto{S^{(w)}} -\psi \] (2.22)
which yields that
\[ U^{(w,\theta)}(\psi - S^{(\theta)} \psi) = (\psi - S^{(\theta)} \psi), \quad \text{and} \quad U^{(w,\theta)}(\psi + S^{(\theta)} \psi) = -(\psi + S^{(\theta)} \psi). \] (2.23)

Note that
\[ S^{(\theta)}(\psi - S^{(\theta)} \psi) = -(\psi - S^{(\theta)} \psi) \in \mathcal{H}_-^{(S)} \quad \text{and} \quad S^{(\theta)}(\psi + S^{(\theta)} \psi) = (\psi + S^{(\theta)} \psi) \in \mathcal{H}_+^{(S)}. \] (2.24)

Since the dimension of the whole space of the DTQW is \(|D| = 2|E|\) and \(\dim(\mathcal{H}_\pm^{(S)}) = |E|\), from Eq. (2.18),
\[ \dim(\mathcal{H}_+^{(S)} \cap \mathcal{L}^\perp) = |E| - (|V| - m_{-1}), \quad \text{and} \quad \dim(\mathcal{H}_-^{(S)} \cap \mathcal{L}^\perp) = |E| - (|V| - m_1). \]

So we obtain for any \( \psi \in \mathcal{H}_+^{(S)} \cap \mathcal{L}^\perp \), \( U^{(w,\theta)} \psi = -\psi \) with the multiplicity \(|E| - |V| + m_{-1}\), and for any \( \psi \in \mathcal{H}_-^{(S)} \cap \mathcal{L}^\perp \), \( U^{(w,\theta)} \psi = \psi \) with the multiplicity \(|E| - |V| + m_1\).

By the way, we should remark that if \( \psi_\pm \in \mathcal{H}_\pm^{(S)} \cap \ker(d_A) \), then it is hold that
\[ d_{B} \psi_\pm(u) = d_{A} S^{(\theta)} \psi_\pm(u) = \pm d_{A} \psi_\pm(u) = 0, \quad (u \in V(G)). \]

Thus \( \psi_\pm \) belongs to also \( \ker(d_B) \). Moreover \( \mathcal{L} = \text{span}\{A, B\} \) implies
\[ \mathcal{L}^\perp = \ker(d_A) \cap \ker(d_B). \]

Therefore \( \mathcal{H}_\pm^{(S)} \cap \ker(d_A) \subseteq \ker(d_A) \cap \ker(d_B) \cap \mathcal{H}_\pm^{(S)} = \mathcal{L}^\perp \cap \mathcal{H}_\pm^{(S)}. \) So we can conclude
\[ \mathcal{H}_\pm^{(S)} \cap \ker(d_A) = M_\pm. \] (2.25)

We complete the proof. \( \square \)

Let \( G \) be a connected graph and \( p : D(G) \to (0, 1] \) a transition probability; that is, \( \sum_{e : o(e) = u} p(e) = 1 \) for all \( u \in V(G) \). If there exists a positive valued function \( m : V(G) \to (0, \infty) \) such that
\[ m(o(e)) p(e) = m(t(e)) p(e), \]
for every \( e \in D(G) \), then \( p \) is said to be reversible, and \( m \) is called reversible measure.
Proposition 2. The random walk on $G$, whose transition probability $p : D(G) \rightarrow [0,1]$ is given by $p(e) = |w(e)|^2$, has the reversible measure if and only if there exists 1-form $\theta$ so that $1 \in \text{spec}(T^{(\theta)})$.

Proof. At first, we show that there exists 1-form $\theta$ so that $1 \in \text{spec}(T^{(\theta)})$ if and only if

$$m(o(e))w(e) = m(t(e))\bar{w}(\bar{e}),$$

(2.26)

respectively. Here $\bar{w}(e) \equiv w(e)e^{i\theta(e)/2}$. This is an extended detailed balanced condition (DBC). The multiplicities of $m_{\pm}$ is positive if and only if the two equalities in Eq. \ref{2.8} holds. Note that the first equality in Eq. \ref{2.8} holds if and only if

$$||\Pi_A S^{(\theta)} \Pi_A \psi||^2 = ||S^{(\theta)} \Pi_A \psi||^2 \iff S^{(\theta)} \Pi_A \psi \in A \iff \Pi_A \psi \in B.$$

On the other hand, the second equality in Eq. \ref{2.8} holds if and only if

$$||\Pi_A \psi||^2 = ||\phi||^2 \iff \psi \in A.$$

Combining these, $|\lambda| = 1$ if and only if $\psi \in A \cap B$. Since $\psi \in A$, using eigenfunction of $T$ for eigenvalue $\lambda = 1$ or $\lambda = -1, m \in \ell^2(V)$, we can express $\psi = d_A^*m$. On the other hand, since $\psi \in B$, there exists $h \in \ell^2(V)$ such that

$$d_B^*h = d_A^*m.$$

Multiplying $d_A$ both sides, we have $h = \pm m$ because of Remark. Thus we have $\lambda = \pm 1$ if and only if

$$d_A^*m = \pm d_B^*m.$$

Inserting the definitions of $d_A^*$ and $d_B^*$ in Eq. \ref{2.2} into Eq. \ref{2.27}, $\lambda = 1$ if and only if

$$m(o(e))w(e) = m(t(e))\bar{w}(\bar{e})e^{-i\theta(e)},$$

(2.28)

for every $e \in D(G)$. Note that this condition is equivalent to the DBC in Eq. \ref{2.26}.

Secondly we show that the DBC is equivalent to that $\{|w(e)|^2 : e \in D(G)\}$ has the reversible measure. Taking its square modulus both sides of Eq. \ref{2.26}, we have the sufficiency. To prove the opposite direction, let us consider a spanning tree $T(G)$ of $G$. We define $C(G)$ as the set of all cycles in $G$. We can give a one-to-one correspondence between a subset of cycle $C^{(0)} \equiv \{c_1, c_2, \ldots, c_r\} \subset C(G)$ and $E(G) \not\subset E(T(G))$, where

$$r = |E(G) \setminus E(T(G))| = |E(G)| - (|V(G)| - 1).$$

(2.29)

Here the cycle $c_j \in C^{(0)}$ is generated by adding edge $e_j \in E(G) \setminus E(T(G))$ to the spanning tree $T(G)$. The subset $C^{(0)}$ is a minimum generator of $C(G)$ in the following meaning; for any $c \in C(G)$, there exist positive integers $\{n_1, n_2, \ldots, n_r\}$ such that $c = \sum_{j=1}^r n_j e_j$. The DBC holds under the assumption that the random walk $\{|w(e)|^2 : e \in D(G)\}$ is reversible if and only if for any cycle $c = \{e_1, \ldots, e_n\} \in C^{(0)}$,

$$m(o(e_1)) = \frac{\bar{w}(e_1)}{w(e_1)} m(o(e_2)) = \frac{\bar{w}(e_1)\bar{w}(e_2)}{w(e_1)w(e_2)} m(o(e_3)) = \cdots = \prod_{j=1}^n \frac{\bar{w}(e_j)}{w(e_j)} m(o(e_1)).$$
Therefore denoting \[ \int_c \text{arg}(\tilde{f}) = \sum_{j=1}^n \left\{ \text{arg}(\tilde{f}(e_j)) - \text{arg}(\tilde{f}(\bar{e}_j)) \right\}, \]
\[ \int_c \text{arg}(\tilde{w}) \in 2\pi\mathbb{Z}. \] (2.30)

For given \( w \), we can adjust \( \theta \) so that Eq. (2.30) holds: for \( c_j = (e_{i_j}^{(j)}, \ldots, e_{k_j}^{(j)}) \in C(0), \)
\[ \theta(e_{i_j}^{(j)}) = \begin{cases} \int_{c_j} \text{arg}(w), & e_{i_j}^{(j)} = e_j, \\ 0, & \text{otherwise}. \end{cases} \] (2.31)

We complete the proof. \( \square \)

Similar to the proof of Proposition 2, we can show that \( \lambda = -1 \) if and only if the signed DBC holds:
\[ m(o(e))\tilde{w}(e) = -m(t(e))\tilde{w}(\bar{e}). \]

Under the above discussions, we consider the following four situations:

(i) \( G \) is bipartite and \( \{|w(e)|^2 : e \in D(G)\} \) is reversible and \( \int_c \text{arg}(\tilde{w}) \in 2\pi\mathbb{Z} \) for any closed path \( c \).

(ii) \( G \) is non-bipartite and \( \{|w(e)|^2 : e \in D(G)\} \) is reversible and \( \int_c \text{arg}(\tilde{w}) \in 2\pi\mathbb{Z} \) for any closed path \( c \).

(iii) \( G \) is non-bipartite and \( \{|w(e)|^2 : e \in D(G)\} \) is reversible and for any closed path \( c, \)
\[ \int_c \text{arg}(\tilde{w}) \in \begin{cases} 2\pi\mathbb{Z} & : \text{c is even length closed path}, \\ 2\pi(\mathbb{Z} + 1/2) & : \text{c is odd length closed path}. \end{cases} \]

(iv) otherwise

These situations are same as the situation appearing in the discussion of the spectrum of twisted random walk on para-line graph in Ref. [7]. According to Ref. [7], we have the following lemma.

**Lemma 1.** Let \( m_{\pm1} \) be the above. Then we have
\[ (m_1, m_{-1}) = \begin{cases} (1,1) & ; \text{case [I]}, \\ (1,0) & ; \text{case [II]}, \\ (0,1) & ; \text{case [III]}, \\ (0,0) & ; \text{case [IV]}. \end{cases} \] (2.32)

From now on, we devote to a special case of twisted Szegedy walk with \( \theta(e) = 0, w(e) = 1/\sqrt{\deg(o(e))} \). This is nothing but the Grover walk. We denote the time evolution of the Grover walk by \( U_{\text{Grover}}^{(u,v)} = U_{\text{Grover}} \). Let \( P \) be the probability transition matrix of the symmetric random walk on \( G \). The symmetric means for any \( u,v \in V(G), \) \( (P)_{u,v} = 1/(\deg(u)). \) It is well known that the reversible distribution of the symmetric random walk \( \pi : V(G) \rightarrow \)
positive integers \(\{n_r\}\). In this setting, we can notice that
\[
T = \mathcal{D}^{-1}P\mathcal{D},
\]
where \(\mathcal{D} = \text{diag}[\sqrt{\pi(u)}; u \in V(G)]\). Thus \(\text{spec}(P) = \text{spec}(T)\), moreover if \(\eta\) is the eigenvector of \(P\), then \(\mathcal{D}^{-1}\eta\) is the eigenvector of \(T\) for the same eigenvalue.

As we will see later, we will characterize the eigenspace of the Grover walk corresponding to \(L^\perp\) in the above lemma by the cycles of \(G\). To do so, let us prepare some new notations. We put the sets of all the essential even and odd cycles are denoted by \(C_e\) and \(C_o\), respectively. Moreover we define \(C_{o-o}\) as the set of Euler closed path consisting of distinct two odd cycles and so called bridge between two cycles, i.e.,
\[
\begin{align*}
C_{o-o} &\equiv \{c = (c_1, p, c_2, p^{-1}) \in P(G) : c_1, c_2 \in C_o(G), p \in \{P_0(G), \emptyset\}, \\
o(c_1) &= t(c_1) = o(p), \quad o(c_2) = t(c_2) = t(p), \quad V(c_1) \cap V(c_2) \subseteq \{\emptyset, o(c_1)\} \}\.
\end{align*}
\]

We define two maps \(\gamma, \tau : P(G) \rightarrow \mathbb{C}^2(D(G))\) by for \(p = (e_1, e_2, \ldots, e_n) \in P(G)\),
\[
\begin{align*}
\gamma(p) &= \sum_{j=1}^{n} (\delta_{e_j} - \delta_{\overline{e_j}}), \quad (2.34) \\
\tau(p) &= \sum_{j=1}^{n} (-1)^j (\delta_{e_j} + \delta_{\overline{e_j}}). \quad (2.35)
\end{align*}
\]

**Theorem 1.** Define the eigenspaces for \(U_{\text{Grover}}\) by
\[
\mathcal{M}_+ = L^\perp \cap H^{(S)}_+ \quad \text{and} \quad \mathcal{M}_- = L^\perp \cap H^{(S)}_-
\]
whose eigenvalue are \(\pm 1\), respectively. Then we have
\[
\begin{align*}
\mathcal{M}_+ &= \sum_{c \in C(G)} \mathbb{C}\gamma(c), \quad (2.36) \\
\mathcal{M}_- &= \sum_{c \in C_e \cup C_{o-o}} \mathbb{C}\tau(c). \quad (2.37)
\end{align*}
\]

Here \(\dim(\mathcal{M}_+) = |E(G)| - |V(G)| + 1\), and \(\dim(\mathcal{M}_-) = |E(G)| - |V(G)| + 1_{(G \text{ is bipartite})}\). In particular, define \(CP_e\) as the set of all even-length closed paths. So we have
\[
\sum_{c \in CP_e} \mathbb{C}\tau(c) = \mathcal{M}_-, \quad \sum_{c \in CP_e} \mathbb{C}\gamma(c) \subset \mathcal{M}_+.
\]

**Proof.** We can easily check from Eqs. \((2.19)\) and \((2.25)\) that for any \(c \in C(G)\), we have \(\gamma(c) \in \mathcal{M}_+\), that is, \(U\gamma(c) = \gamma(c)\). Let \(C^{(0)}\) be the above. For any \(c \in C(G)\), there exist positive integers \(\{n_1, n_2, \ldots, n_r\}\) such that \(\gamma(c) = \sum_{j=1}^{n_r} n_j\gamma(c_j)\). Therefore we arrive at \(\mathcal{M}_+ = \text{span}\{\gamma(c); c \in C^{(0)}\} = \text{span}\{\gamma(c); c \in C(G)\}\).

In the next step, from Eqs. \((2.19)\) and \((2.25)\), for any \(c \in C_e(G) \cup C_{o-o}\), we also confirm \(\tau(c) \in \mathcal{M}_-\), that is, \(U\tau(c) = -\tau(c)\). Note that \(C^{(0)} \subseteq C_e(G)\) iff the graph is bipartite. In this case, \(\mathcal{M}_- = \text{span}\{\tau(c) : c \in C^{(0)}\}\). Now we consider the case that \(C^{(0)}\) has odd
cycles. Assume that $c_1, \ldots, c_K$ are odd cycles and $c_{K+1}, \ldots, c_r$ are even cycles ($K \leq r$). Remark that for any cycle $c_i, c_j \subset C_o(G)$, there exists a simple path $p_{i,j} \in P_0(G)$ such that $(c_i, p_{i,j}, c_j, p^{-1}_{i,j}) \subset C_{o-o}$. Then

$$\mathcal{M}_- = \text{span}\{\{\tau(c_1,p_{1,j},c_j,p^{-1}_{1,j}) : 2 \leq j \leq K\} \cup \{\tau(c_j) : K < j \leq r\}\}. \quad (2.38)$$

Since all the $\tau(c_1,p_{1,j},c_j,p^{-1}_{1,j})$ ($2 \leq j \leq K$) and $\tau(c_j)$ ($K+1 \leq j \leq r$) are linearly independent, we have

$$\text{dim}(\mathcal{M}_-) = K - 1 + (r - K) = |E| - |V|.$$ 

We can easily check that $\tau(p) \in \mathcal{M}_-$ and $\gamma(p) \in \mathcal{M}_+$ for any $p \in CP_e$. Since $C_{o-o}, C_e \subset CP_e$, we obtain the conclusion. We complete the proof. \hfill \Box

## 3 Grover walk on crystal lattice

### 3.1 Setting

Define a partition $\pi : G \rightarrow G^{(o)} = (V^{(o)}, D^{(o)})$ satisfying the following conditions:

1. $V^{(o)} = \pi(V(G)) = \{V_1, V_2, \ldots, V_r\}$ with $V_i \cap V_j = \emptyset$ ($i \neq j$).
2. for $e \in D(G)$, $\pi(o(e)) = o(\pi(e))$ and $\pi(t(e)) = t(\pi(e))$.
3. $D_u \xrightarrow{\gamma} D_{\pi(u)}$: bijection, where $D_u = \{e \in D(G) : o(e) = u\}$.

**Remark 4.** Under the assumption of (3), $\deg(u) = \deg(\pi(u))$ for all $u \in V(G)$. In particular, if there exists an abelian operator $\Gamma \subset \hat{C}P_e$, then $G$ is called crystal lattice. We take a spanning tree $T^{(o)}$ of $G^{(o)} = \Gamma \setminus G$. Let $E(G^{(o)}) \setminus E(T^{(o)}) = \{e_1, \ldots, e_r\}$. We assign 1-form $\theta$ so that $\theta(e) = 0$ iff $e \in D(T^{(o)})$. Prepare $r$ vectors $\hat{\theta}_1, \ldots, \hat{\theta}_r \in \mathbb{R}^d$ ($d \leq r$). Here $r = |E(G^{(o)}) \setminus E(T^{(o)})|$. We will put $\theta(e_j) = -\theta(e_j) = \langle k, \hat{\theta}_j \rangle$ for $k \in \mathbb{R}^d$ and $e_j \in E(G^{(o)} \setminus T^{(o)})$ in the later discussion.

To construct a crystal lattice $G = (V, D)$, we start from a finite graph $G^{(o)} = (V^{(o)}, D^{(o)})$. Prepare $r$-unit vector $\hat{\theta}_1, \ldots, \hat{\theta}_r \in \mathbb{R}^d$ ($d \leq r$). We assume $\text{rank}[\hat{\theta}_1, \ldots, \hat{\theta}_r] = d$. At first, we put copies of the quotient graph $G^{(o)}$ on every lattice $L = \mathbb{Z}\hat{\theta}_1 + \cdots + \mathbb{Z}\hat{\theta}_r \subset \mathbb{R}^d$. The vertex $u$ of $G^{(o)}$ at $x \in L$ is labeled by $(x, u)$ here. Let $T^{(o)}$ be a spanning tree of $G^{(o)}$. Secondly, each terminus of arc $e_j \in D(G^{(o)} \setminus T^{(o)})$ at $x \in L$ is rewired to the terminus of the neighbor located in $x + \hat{\theta}_j$; that is, if $t(e_j) = (x, v)$ in the first step, then, $t(e_j)$ is changed to $(x + \hat{\theta}_j, v)$ in the second step. We take this procedure to every lattice $x \in L$. From this, we obtain a covering graph $G$. In particular, when the transformation group $\Gamma$ with $G^{(o)} = \Gamma \setminus G$ is the 1-homology group $H_1(G^{(o)}, \mathbb{Z})$, $G$ is called maximal abelian covering graph of $G^{(o)}$. In
other words, when \( \{ \hat{\theta}_j \}_{j=1}^r \) are linearly independent, then \( G \) is the maximal abelian covering graph. So we will consider the Grover walk on the 1-homology group \( H_1(G^{(o)}, \mathbb{Z}) \).

Given a crystal lattice \( G = (V, D) \), \( V(G) \) and \( D(G) \) are isomorphic to \( L \times V^{(o)} \) and \( D(G) = L \times D^{(o)} \), respectively. From now on, we use both \( I(G) \) and \( L \times I^{(o)} \) depending on the situation \( (I \in \{ V, D, E \}) \). Define for \( u \in V(G) \), \( \mathcal{H}_u = \{ \delta_e; o(e) = u \} \subset \ell^2(D(G)) \). Recall that the time evolution is \( U = SC \). The coin operator \( C \) is rewritten by \( \bigoplus_{u \in V(G)} H_u \). Here \( H_u \) is so called the Grover coin operator on \( \mathcal{H}_u \) assigned at vertex \( u \):

\[
(H_u)_{e,f} = 1_{\{ o(e) = o(f) = u \}} \left( \frac{2}{\deg(u)} - \delta_{e,f} \right).
\]

We assume that \( (H_u)_{e,f} = (H_{\sigma(u)})_{\sigma(e),\sigma(f)} \equiv (H_{\pi(u)})_{e_o,f_o} \) for any \( e \in \pi^{-1}(e_o) \), \( f \in \pi^{-1}(f_o) \), and \( \sigma \in \Gamma \). Define for \( e \in D \), \( P_e : \mathcal{H}_{o(e)} \rightarrow \mathcal{H}_{t(e)} \) associated with a “move” from \( o(e) \) to \( t(e) \) such that

\[
P_e = \Pi_{\delta_k} U \Pi_{H_u(e)}
\]

Let \( \Psi_n : L \times V^{(o)} \rightarrow \ell^2(L \times D^{(o)}) \) at time \( n \in \mathbb{N} \) be denoted by \( \Psi_n(x, v) = \Pi_{\mathcal{H}_v} U^n \Psi_0 \). Here \( \Psi_0 \in \ell^2(L \times D^{(o)}) \) is the initial state. We can observe that

\[
\Psi_n(x, v) = \sum_{f \in D^{(o)}; t(f) = v} P_f \Psi_{n-1} \left( x - \hat{\theta}(f), o(f) \right).
\]

(3.39)

where \( \hat{\theta}(f) = 0 \) if \( f \in E(T^{(o)}) \), \( \hat{\theta}(f) = \hat{\theta}_j \) if \( f = e_j \in E(G^{(o)} \setminus T^{(o)}) \) \( (j \in \{1, \ldots, r\}) \). We define the finding distribution \( \nu_n : V(G) \rightarrow [0, 1] \) by

\[
\nu_n(x, v) = |\Psi_n(x, v)|^2.
\]

We denote a random variable \( X_n \) following \( P(X_n = x) = \mu(x) \equiv \sum_{v \in V^{(o)}} \nu_n(x, v) \). Our interest will be the sequence of \( \{ \mu_n \}_{n \in \mathbb{N}} \) in this paper.

### 3.2 Spectrum

Let the Fourier transform \( \mathcal{F} : L^2(K^d \times D^{(o)}) \rightarrow \ell^2(L \times D^{(o)}) \) be

\[
(\mathcal{F} g)(x, f) = \int_{0}^{2\pi} g(k, f) e^{-i(k,x)} \frac{d \ell}{(2\pi)^d}.
\]

Here \( K = [0, 2\pi) \). So the dual operator \( \mathcal{F}^* : \ell^2(L \times D^{(o)}) \rightarrow L^2(K^d \times D^{(o)}) \) is described by

\[
(\mathcal{F}^* \phi)(x, f) = \sum_{x \in L} \phi(x, f) e^{i(k,x)}.
\]

Taking \( \mathcal{F}^* \) to both sides of Eq. (3.39), we have

\[
\tilde{\Psi}_n(k, v) = \sum_{f : t(f) = v} e^{i(k, \hat{\theta}(f))} P_f \tilde{\Psi}_{n-1}(k, o(f)).
\]

(3.40)
Here $\widetilde{\Psi}_n(k, v) = F^*\Psi_n(x, v)$. Define $\widetilde{U}^{(o)}_k$ as the twisted Szegedy walk $U^{(w, \theta)}$ on the quotient graph $G^{(o)}$ with

$$w(e) = 1/\sqrt{\deg(o(e))}, \quad \theta(e) = (k, \hat{\theta}(e)) \quad (e \in D^{(o)}).$$

(3.41)

Here $\hat{\theta}(e) = 0$ if $e \in T^{(o)}$. We also denote the discriminant operator of $\widetilde{U}_k^{(o)}$ by $\hat{T}_k^{(o)} \equiv T^{(w, \theta)}$ with the above $w$ and $\theta$.

The important statement of this section is that the Grover walk on $G$ is reduced to the twisted Szegedy walk on the quotient graph $G^{(o)}$ in the Fourier space as follows:

$$\widetilde{\Psi}_n(k, v) = \Pi_{\mathcal{H}_w} \left( \widetilde{U}^{(o)}_k \right)^n \sum_{u \in V^{(o)}} \widetilde{\Psi}_0(k, u).$$

(3.42)

In other words, taking $U_{\text{Grover}}$ as the time evolution of the Grover walk on the maximal abelian covering graph $G^{(o)}$, for any $\widetilde{\Psi}_0 \in L^2(K^d \times D^{(o)})$,

$$F[\{\widetilde{U}^{(o)}_k\}^n \widetilde{\Psi}_0] = U^n_{\text{Grover}} F[\widetilde{\Psi}_0].$$

(3.43)

By the way, let $Y_n^{(u)} \in L \times V^{(o)}$ be a simple random walk at time $n$ on $G$ starting from $(0, u)$. Denote the characteristic function of $Y_n^{(u)}$ by for $k \in K^d$,

$$\chi_n(k; u, v) \equiv \sum_{x \in L} P(Y_n^{(u)} = (x, v)) e^{i(k, x)}.$$

Let $|V^{(o)}| \times |V^{(o)}|$ matrix $\widetilde{P}^{(o)}_k$ for $u, v \in V^{(o)}$ be $\left( \widetilde{P}^{(o)}_k \right)_{u, v} = \chi_1(k; u, v)$. Then

$$\chi_n(k; u, v) = \left( \left\{ \widetilde{P}^{(o)}_k \right\} \right)_{u, v}.$$

A relation between $\hat{T}_k^{(o)}$ and $\hat{P}^{(o)}_k$ is

$$\hat{T}_k^{(o)} = \mathcal{D}^{-1} \hat{P}^{(o)}_k \mathcal{D},$$

(3.44)

where $\mathcal{D}$ is given by Eq. (2.33) inserting the square root of the stationary distribution of simple random walk on $G^{(o)}$; that is, $\sqrt{\pi}(u) = 1/\sqrt{\deg(u)}$ for all $u \in V^{(o)}$.

**Proposition 3.** Let $\hat{P}^{(o)}_k$ be defined by the above. When $k \in \mathbb{R}^d$ satisfies $(k, \hat{\theta}(e)) \notin \pi\mathbb{Z}$, for some $e \in D^{(o)}$, then we have

$$\text{spec}(\hat{U}^{(o)}_k) = \varphi^{-1}_{QW}(\text{spec}(\hat{P}^{(o)}_k)) \cup \{1\}^{\{E^{(o)}\} - |V^{(o)}|} \cup \{-1\}^{\{E^{(o)}\} - |V^{(o)}|}.$$

**Proof.** From Eq. (3.44), we have $\text{spec}(\hat{T}^{(o)}_k) = \text{spec}(\hat{P}^{(o)}_k)$, and the relation between eigenfunctions $\rho$ and $\rho'$ of the eigenvalue for $\hat{T}^{(o)}_k$ and $\text{spec}(\hat{P}^{(o)}_k)$ is $\rho' = \mathcal{D} \rho$. Therefore we can directly applying Lemma 1. On the other hand, obviously the assumption that $(k, \hat{\theta}(e)) \notin \pi\mathbb{Z}$, for some $e \in D^{(o)}$ leads to the case of (iv). From Lemma 1 $m_{\pm 1} = 0$; that is, the multiplicities of $\pm 1$ are $M_{\pm 1} = |E^{(o)}| - |V^{(o)}|$, respectively. We arrive at the conclusion. \qed
Let the eigenspace of eigenvalues \( \varphi_{\omega}^{-1}(\text{spec}(\check{\mathcal{T}}^{(o)}_k)) \) be \( \check{\mathcal{L}}^{(o)}_k \subset L^2(K^d \times D^{(o)}) \). We denote \( \check{S}^{(o)}_k : L^2(K^d \times D^{(o)}) \to L^2(K^d \times D^{(o)}) \) by \( \check{S}^{(o)}_k f(k,e) = e^{-i(k,\check{\theta}(c))} f(k,e) \). Remark that \( \check{S}^{(o)}_k \) has two eigenvalues \( \pm 1 \). We put the eigenspaces of eigenvalues \( \pm 1 \) for \( \check{S}^{(o)}_k \) as \( \check{\mathcal{H}}^{(o)}_{\pm} \). Define \( \check{\mathcal{M}}^{(o)}_{\pm} = \check{\mathcal{L}} \cap \check{\mathcal{H}}^{(o)}_{\pm} \).

**Proposition 4.** For given graph \( G^{(o)} \) with the quotient graph \( G^{(o)} \), let \( \mathcal{M}_{\pm} \subset \ell^2(L \times D^{(o)}) \) be defined by Eqs. (2.36) and (2.37), respectively. It is hold that

\[
\sum_{x \in L} C \mathcal{F}(e^{i(k,x)} \check{\mathcal{M}}^{(o)}_{\pm}) = \mathcal{M}_{\pm}
\]

**Proof.** At first, we will prove that \( \mathcal{M}_{\pm} \subset \sum_{x \in L} C \mathcal{F}(e^{i(k,x)} \check{\mathcal{M}}^{(o)}_{\pm}) \). Remark that closed cycle in \( G, c = (f_1, f_2, \ldots, f_k) \) with \( f_j = (x_j, e_j) (x_j \in L, e_j \in D^{(o)}) \), is represented by closed path \( (e_1, \ldots, e_\kappa) \) in \( G^{(o)} \). Note that

\[
\check{f}_j = (x_j + \check{\theta}(e_j), \bar{e}_j) \quad \text{and} \quad f_{j+1} = (x_j + \check{\theta}(e_j), e_{j+1}).
\]

It is hold that

\[
(F^*\gamma(c))(k, \bar{e}_j) = -e^{i\theta(e_j)}(F^*\gamma(c))(k, e_j), \quad (1 \leq j \leq \kappa) \quad (3.45)
\]

\[
(F^*\gamma(c))(k, e_{j+1}) = e^{i\theta(e_j)}(F^*\gamma(c))(k, e_j), \quad (1 \leq j \leq \kappa) \quad (3.46)
\]

Here we take \( \theta(e_j) = \langle k, \check{\theta}(e_j) \rangle \). (See Eq. (3.41).) From Eqs. (3.45) and (3.46), we have

\[
(F^*\gamma(c))(k, \bar{e}_\kappa) = -\exp\left[ i \int_{(e_1, \ldots, e_\kappa)} \theta \right] (F^*\gamma(c))(k, e_1)
\]

Since \( c \) is closed cycle of \( G \), we have \( \int_{(e_1, \ldots, e_\kappa)} \theta = 0 \) which leads to

\[
\sum_{f : o(f) = o(e_j)} (F^*\gamma(c))(f) = 0, \quad (1 \leq j \leq \kappa). \quad (3.47)
\]

By the way, equation (3.47) implies

\[
F^*\gamma(c) \in \check{\mathcal{H}}^{(o)}_{-}.
\]

Combining Eq. (3.47) with Eq. (3.48), from Eq. (2.25), \( F^*\gamma(c) \in \check{\mathcal{M}}^{(o)}_{\pm} \). In the same way, for any even-length closed path \( c \) in \( G \), we have \( F^*\tau(c) \in \check{\mathcal{M}}^{(o)}_{\pm} \). So we arrive at \( \mathcal{M}_{\pm} \subset \sum_{x \in L} C \mathcal{F}(e^{i(k,x)} \check{\mathcal{M}}^{(o)}_{\pm}) \).

From now on, we will prove \( \mathcal{M}_{\pm} \subset \sum_{x \in L} C \mathcal{F}(e^{i(k,x)} \check{\mathcal{M}}^{(o)}_{\pm}) \). The set of cycles \( C^{(o)} = \{ c_1, \ldots, c_r \} \) with \( r = |E^{(o)}| - |V^{(o)}| + 1 \) represents \( E(G^{(o)} \setminus \mathbb{T}^o) \). We put \( c_j = (e_{1j}, \ldots, e_{\kappa j}) \) so that \( \theta(e_{1j}) = \theta_j (j \in \{1, \ldots, r \}) \). Remark that \( \theta(e_{1i}) = 0 \) for \( i \neq 1 \). For the pair of \( c_1 \) and \( c_j \), we can take a path \( P = (f_1, \ldots, f_\ell) \) so that \( o(P) = o(c_1) \) and \( t(P) = o(c_j) \). Let a new closed path \( \check{c}_1 \) and \( \check{c}_j \) be for \( 1 \leq \kappa \leq l \)

\[
\check{c}_1 = (f_\kappa, \check{f}_\kappa - 1, \ldots, \check{f}_1, e_{11}^{(1)}, \ldots, e_{n1}^{(1)}, f_1, \ldots, f_{\kappa-1}, f_\kappa)
\]

\[
\check{c}_j = (f_{\kappa+1}, f_{\kappa+2}, \ldots, f_\ell, e_{1j}^{(j)}, \ldots, e_{nj}^{(j)}, \check{f}_1, \check{f}_1 - 1, \ldots, \check{f}_{\kappa+1}).
\]
respectively. Define \( \eta_j, \zeta_j \in \ell^2(D^{(o)}) \) by

\[
\begin{aligned}
\eta_1(e) &= \begin{cases} 
(-1)^{\kappa-m} ; e = \tilde{f}_m, 1 \leq m \leq \kappa \\
(-1)^\kappa ; e = e_1^{(1)} \\
(-1)^{\kappa+m-1}e^{i\theta_1} ; e = e_m^{(1)}, 2 \leq m \leq n_1 , \\
(-1)^{\kappa+n_1-1+m}e^{i\theta_1} ; e = f_m, 1 \leq m \leq \kappa \\
0 ; \text{ otherwise}
\end{cases} \\
\zeta_1(e) &= \begin{cases} 
1 ; e = \tilde{f}_m, 1 \leq m \leq \kappa \text{ or } e = e_1^{(1)} \\
e^{i\theta_1} ; e = e_m^{(j)}, 1 \leq m \leq n_j \text{ or } e = f_s, 1 \leq s \leq \kappa \\
0 ; \text{ otherwise}
\end{cases}
\end{aligned}
\]

For \( 2 \leq j \leq r \),

\[
\begin{aligned}
\eta_j(e) &= \begin{cases} 
(-1)^{m-\kappa-1} ; e = f_m, \kappa + 1 \leq m \leq l \\
(-1)^{l-\kappa} ; e = e_1^{(j)} \\
(-1)^{l-\kappa+m-1}e^{i\theta_j} ; e = e_m^{(j)}, 2 \leq m \leq n_j , \\
(-1)^{l-\kappa+n_j+(l-m)}e^{i\theta_j} ; e = f_m, \kappa + 1 \leq m \leq l \\
0 ; \text{ otherwise}
\end{cases} \\
\zeta_j(e) &= \begin{cases} 
1 ; e = f_m, \kappa + 1 \leq m \leq l \text{ or } e = e_1^{(j)} \\
e^{i\theta_j} ; e = e_m^{(j)}, 1 \leq m \leq n_j \text{ or } e = f_s, \kappa + 1 \leq s \leq l \\
0 ; \text{ otherwise}
\end{cases}
\end{aligned}
\]

We can notice that taking \( Q_{\pm} \equiv I \pm S^{(\theta)} \), for \( u \in V(\tilde{c}_j) \),

\[
\sum_{e:o(e)=u} Q_+ \eta_j(e) = \begin{cases} 
1 - (-1)^{n_j}e^{i\theta_j} ; u = o(\tilde{c}_j) \\
0 ; \text{ otherwise}
\end{cases} \quad (3.49)
\]

\[
\sum_{e:o(e)=u} Q_- \zeta_j(e) = \begin{cases} 
1 - e^{i\theta_j} ; u = o(\tilde{c}_j) \\
0 ; \text{ otherwise}
\end{cases} \quad (3.50)
\]

Moreover since \( S^{(\theta)}Q_{\pm} = \pm Q_{\pm}, Q_+ \eta \in \tilde{H}_+^{(o)} \) and \( Q_- \eta \in \tilde{H}_-^{(o)} \). From these observations, we define \( \tilde{\eta}_j \) and \( \tilde{\zeta}_j \) instead of \( \eta \) and \( \zeta \) as follow so that \( \tilde{\eta}_j, \tilde{\zeta}_j \in \ker(d^{(}\lambda)): \)

\[
\begin{aligned}
\tilde{\eta}_j &= (1 - (-1)^{n_j}e^{i\theta_j}) Q_+ \eta_j - (1 - (-1)^{n_j}e^{i\theta_j}) Q_+ \eta_1, \quad (3.51) \\
\tilde{\zeta}_j &= (1 - e^{i\theta_j}) Q_- \zeta_j - (1 - e^{i\theta_j}) Q_- \zeta_1. \quad (3.52)
\end{aligned}
\]

Thus Eq. (2.23) implies \( \tilde{\eta}_j \in \tilde{M}_-^{(o)}, \tilde{\zeta}_j \in \tilde{M}_+^{(o)} \), respectively. Since the functions \( \{\tilde{\eta}_j\}_j \) and \( \{\tilde{\zeta}_j\}_j \) are linearly independent and the situation is case (iv) for almost all \( k \in \mathbb{R}^d \), it is hold that \( \tilde{M}_-^{(o)} = \text{span}\{\tilde{\eta}_j; j \in \{1, \ldots, r\}\} \) and \( \tilde{M}_+^{(o)} = \text{span}\{\tilde{\zeta}_j; j \in \{1, \ldots, r\}\} \) a.e. We can confirm that for the pair of closed paths \( \tilde{c}_1 \) and \( \tilde{c}_2 \) in \( G^{(o)} \), there exists a finite closed path \( p \) of even length in \( G \) such that \( \mathcal{F}\tilde{c}_j = \gamma(p) \) and \( \mathcal{F}\tilde{\eta}_j = \tau(p) \). From Theorem 1 we have

\[
\sum_{x \in L} \mathbb{C}\mathcal{F}(e^{i(k,x)}\tilde{M}_\pm^{(o)}) \subset \mathcal{M}_\pm.
\]

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Let \( P_G : D(V) \times D(V) \to [0, 1] \) be the stochastic operator of a simple random walk on crystal lattice \( G \); that is,
\[
P_G(u, v) = 1_{(u, v) \in D(G) / \deg(u)}.
\]
Let \( U(G) \) be the time evolution of the Grover walk on \( G \). As a consequence of Propositions 3 and 4, we have the following corollary.

**Corollary 1.** Let
\[
N = \begin{cases} 
\infty & ; \text{G has cycles,} \\
0 & ; \text{otherwise.}
\end{cases}
\]
Then we have
\[
\text{spec}(U(G)) = \varphi^{-1}_{QW}(P(G)) \cup \{1\}^N \cup \{-1\}^N
\]

### 3.3 Stochastic behaviors

Here we define specific properties of the quantum walk, called localization and linear spreading:

1. Localization occurs if and only if there exists \( x \in L \) such that
\[
\lim \sup_{n \to \infty} \mu_n(x) > 0.
\]
2. Linear spreading happens if and only if
\[
\lim_{n \to \infty} \sum_{x \in L} ||x/n||^2 \mu_n(x) \in (0, \infty)
\]

From now on, we define
\[
\Phi^{(o)} = \{ \phi : \mathbb{R}^d \to \mathbb{R}^d : \cos \phi(k) \in \tilde{P}_{k}^{(o)} \}
\]
and eigenfunction of eigenvalue \( \cos \phi \) with \( \phi \in \Phi^{(o)} \) be \( \omega_\phi \in L^2(K^d \times V^{(o)}) \) with \( ||\omega_\phi||^2 = 1 \).

We put the set of arccos’s of the constant eigenvalues
\[
\Lambda = \{ \phi \in \Phi^{(o)} : \partial \phi(k)/\partial k_1 = \partial \phi(k)/\partial k_2 = \cdots = \partial \phi(k)/\partial k_d = 0, \text{ for all } k \in K^d \} = \{ \pm \alpha_1, \ldots, \pm \alpha_s \}, \text{ (} 0 \leq s \leq |V^{(o)}| \).
\]

Here \( s = 0 \) means \( \Lambda = \emptyset \). Let \( S_\phi \) be the set of all critical points of \( \phi \in \Phi^{(o)} \setminus \Lambda \) on \( K^d \); that is, \( \partial \phi|_{S_\phi} = 0 \). Our strategy to show the above properties is based on the stationary phase method. We impose the following natural assumption to \( S_\phi \):

**Assumption.** For every \( \phi \in \Phi^{(o)} \setminus \Lambda \),

(a) both \( \phi(k) \) and eigenfunction \( w_\phi(k, e) \) of eigenvalue \( e^{i\phi(k)} \) are analytic on a neighbor of \( S_\phi \).
(b) each critical point \( p \in S_\phi \) is non-degenerate; that is, its Hessian matrix at \( p \) is invertible.

Here the Hessian matrix of \( \phi \) at \( p \) is defined by

\[
(Hess_\phi(p))_{l,m} = \left. \frac{\partial}{\partial k_l \partial k_m} \phi(k) \right|_{k=p}.
\]

The following lemma corresponding to stationary phase method holds. See for example [13, 16].

**Lemma 2.** Let \( \psi \) and \( \phi \) with \( \text{Re}(\phi) \geq 0 \) be complex-valued analytic functions on a compact neighborhood \( N \) of the origin in \( \mathbb{R}^d \). Suppose that \( \phi \) has only one critical point which is non-degenerate at \( k_0 \). Then we have for sufficient large \( \lambda \),

\[
\int_N e^{\lambda \phi(k)} \psi(k) dk \sim \frac{(2\pi/\lambda)^{d/2} \psi(k_0) e^{i\lambda \phi(k_0)}}{\sqrt{\text{Hess}_\phi(k_0)}}
\]

Here the choice of signature of the square root is decided by taking the number of positive minus the number of negative eigenvalues of \( \text{Hess}_\phi(k_0) \). If \( \phi \) has no critical points on the domain, then \( \int_N e^{\lambda \phi(k)} \psi(k) dk = O(\lambda^{-N}) \) for any \( N > 0 \).

We can provide \( \mathbb{Z}^d \), triangular lattice and hexagonal lattice as typical examples of the crystal lattice. We show that all of the three examples satisfy assumptions (a) and (b) in Appendix. In spite of the above each individual case, the detailed general properties of \( \Phi^{(o)}(\circ) \) remains an interesting future’s problem in this paper. Thus we should remark that there are possibilities that the above assumptions dose not hold in general. In the discrete-time quantum walk on triangular lattice proposed by Ref. [10] but not included by our quantum walk proposed in this paper, due to the degenerate critical point in this walk, the decay rate of the return probability becomes slow down; \( p_n \propto n^{-4/3} \) for large time step \( n \), comparing with the non-degenerate critical point case \( p_n \propto n^{-2} \). It is suggested that the spreading rate is less than one.

By using Lemma 2 we have the following theorem related to the localization.

**Theorem 2.** Under assumptions (a) and (b), if the quotient graph \( G^{(o)} \) satisfies with \( |E^{(o)}| - |V^{(o)}| \geq 1 \) or the discriminant operator \( \bar{T}^{(o)}_k \) has a constant eigenvalue with respect to \( k \in \mathbb{R}^d \), then an appropriate choice of the initial state provides localization of the Grover walk on \( G \).

**Proof.** Suppose that the initial state of the Grover walk on crystal lattice \( G \) is \( \Psi_0 \in \ell^2(L \times D^{(o)}) \) and \( \mathcal{F}^* \Psi_0 = \widetilde{\Psi}_0(k) \). Taking \( \mathcal{F} \) to \( \widetilde{\Psi}(k,u) \),

\[
\Psi_n(x,u) = \int_0^{2\pi} e^{-i(k,x)} \widetilde{\Psi}_n(k,u) \frac{dk}{(2\pi)^d}
\]

Define \( \widetilde{\Psi}_n(k) \equiv \sum_{u \in V^{(o)}} \widetilde{\Psi}_n(k,u) \). From Lemma 1 and Eq. (3.42), we have

\[
\widetilde{\Psi}_n(k) = \sum_{\phi \in \Phi^{(o)} \setminus \Lambda} e^{i\phi(k)} \Pi_{\omega_\phi} \widetilde{\Psi}_0(k) + \sum_{\alpha \in \Lambda} e^{i\alpha \alpha} \Pi_{\omega_\alpha} \widetilde{\Psi}_0(k) + \left( \Pi_{\lambda^+_\varphi} + (-1)^{\alpha} \Pi_{\lambda^-_{\varphi}} \right) \widetilde{\Psi}_0(k). \tag{3.54}
\]
Define $\Psi_n(x) = \sum_{u \in V^{(o)}} \Psi_n(x, u)$. Taking $F$ to both sides of Eq. (3.54),

$$
\Psi_n(x) = \sum_{\phi \in \Phi^{(o)} \setminus \Lambda} \int_0^{2\pi} d\omega_0 \exp\{i\omega_0 (\Phi - (x/n))\} \Pi_{\omega_0} \tilde{\Psi}_0(k) \frac{dk}{(2\pi)^d}
$$

$$
+ \sum_{\alpha \in \Lambda} e^{i\alpha} \int_0^{2\pi} d\omega_0 \exp\{-i(k \cdot x)\} \Pi_{\omega_0} \tilde{\Psi}_0(k) \frac{dk}{(2\pi)^d}
$$

$$
+ \int_0^{2\pi} d\omega_0 \exp\{-i(k \cdot x)\} \left( \Pi_{\hat{M}_+^{(o)}} + (-1)^n \Pi_{\hat{M}_-^{(o)}} \right) \tilde{\Psi}_0(k) \frac{dk}{(2\pi)^d}. \quad (3.55)
$$

Lemma 2 yields that the first term is vanished in the limit of large $n$. Then we have for large time step $n$,

$$
P(X_n^{(\Psi_0)} = x) \sim \left| \int_0^{2\pi} d\omega_0 \exp\{-i(k \cdot x)\} \left( \sum_{\alpha \in \Lambda} e^{i\alpha} \Pi_{\omega_0} + \Pi_{\hat{M}_+^{(o)}} + (-1)^n \Pi_{\hat{M}_-^{(o)}} \right) \tilde{\Psi}_0(k) \frac{dk}{(2\pi)^d} \right|^2. \quad (3.56)
$$

Thus appropriate initial state $\Psi_0$ satisfying $\tilde{\Psi}_0(k) \notin (\mathbb{C}\hat{M}_+^{(o)} + \mathbb{C}\hat{M}_-^{(o)} + \sum_{\alpha \in \Lambda} \mathbb{C}\omega_0)_{\perp}$ provides localization. In particular, in the case of $|E^{(o)}| - |V^{(o)}| \geq 1$, since $\hat{M}_+^{(o)} \neq \emptyset$ holds, then from Proposition 4 if we choose the initial state $\Psi_0 \in \ell^2(L \times D^{(o)})$ so that $\Psi_0 \notin \text{span}\{M_+, M_-\}_{\perp}$, it is ensured that

$$
\limsup_{n \to \infty} P(X_n^{(\Psi_0)} = j) > 0.
$$

Then we obtain the desired conclusion. \(\square\)

**Remark 5.** The crystal lattice proposed by \(\mathcal{F}\) in Sect. 2.2 depicted by Fig. 1 is one of the examples that $|E^{(o)}| - |V^{(o)}| = 0$ but localization occurs.

![Figure 1](image.png)

**Figure 1:** Example of the graph in which $|E^{(o)}| - |V^{(o)}| = 0$ but $T_{k}^{(o)}$ has a constant eigenvalue. $G$ is the original graph and $G^{(o)}$ is its quotient graph.

Finally we consider the contribution of $\Phi^{(o)} \setminus \Lambda$ to the behavior of the Grover walk. To do so, we take a scaling $X_n/n$.

**Lemma 3.** Let the initial state be $\Psi_0 \in \mathcal{H}$ and its Fourier transform be $\tilde{\Psi}_0$. Then we have under the assumptions (a) and (b),

$$
\lim_{n \to \infty} E[e^{i\xi \cdot X_n}/n] = c_0 + \int_{k \in [0,2\pi)^d} \sum_{\phi \in \Phi^{(o)}} e^{i\xi \cdot \nabla_0} ||\Pi_{\omega_0} \tilde{\Psi}_0(k)||^2 \frac{dk}{(2\pi)^d}. \quad (3.57)
$$
Here

\[ c_0 = \int_{0}^{2\pi} \sum_{\alpha \in \Lambda} \left\| \Pi_{\omega_{\alpha}} \tilde{\Psi}_0(k) \right\|^2 \frac{dk}{(2\pi)^d} + \left\| (\Pi_{M_+} + \Pi_{M_-}) \Psi_0 \right\|^2. \]

Proof. The definitions of the spatial Fourier transform and the characteristic function for \( X_n \) provide

\[ E[e^{i(\xi, X_n)}] = \int_{\mathbb{R}^d} \langle \tilde{\Psi}_n(k), \tilde{\Psi}_n(k + \xi) \rangle \frac{dk}{(2\pi)^d}. \] (3.58)

Replacing \( \xi \) with \( \xi/n \) and taking the Taylor expanding to \( \phi \in \Psi_o \), \( \phi(k + \xi/n) = \phi(k) + \langle \xi/n, \nabla \phi(k) \rangle + O(1/n^2) \), and to the eigenfunctions \( \omega_\phi(k + \xi/n, e) = \omega_\phi(k, e) + O(1/n) \), we insert Eq. (3.54) into Eq. (3.58). All the cross terms with respect to the inner product of the integrand in Eq. (3.58) are \( O(1/n) \) from Lemma 2, and the diagonal terms remain as follows:

\[ \sum_{\phi \in \Psi_o} e^{i(\xi, \nabla \phi)} \left\| \Pi_{\omega_\phi} \tilde{\Psi}_0(k) \right\|^2 + \left\| \Pi_{M_+} \tilde{\Psi}_0(k) \right\|^2 + \left\| \Pi_{M_-} \tilde{\Psi}_0(k) \right\|^2 + \sum_{\alpha \in \Lambda} \left\| \Pi_{\omega_{\alpha}} \tilde{\Psi}_0(k) \right\|^2. \]

Remark that the integral of the second term \( \left\| \Pi_{M_+} \tilde{\Psi}_0(k) \right\|^2 \) is rewritten by

\[ \int_{0}^{2\pi} \left\| \Pi_{M_+} \tilde{\Psi}_0(k) \right\|^2 \frac{dk}{(2\pi)^d} = \sum_{x \in L} \left| \int_{0}^{2\pi} \Pi_{M_+} \tilde{\Psi}_0(k) e^{-i(x,k)} \frac{dk}{(2\pi)^d} \right|^2 \]

\[ = \sum_{x \in L} \left| \Pi_x \Pi_{M_+} \Psi_0 \right|^2 \]

\[ = \left| \Pi_{M_+} \Psi_0 \right|^2. \]

Here we use Proposition 4 to the second equality. In the same way, the integral of the third term becomes

\[ \int_{0}^{2\pi} \left\| \Pi_{M_-} \tilde{\Psi}_0(k) \right\|^2 \frac{dk}{(2\pi)^d} = \left| \Pi_{M_-} \Psi_0 \right|^2. \]

Then we complete the proof. \( \square \)

Theorem 3. The Grover walk on the crystal lattice \( G \) under the assumptions (a) and (b) exhibits linear spreading.

Proof. From Lemma 3 we immediately obtain the conclusion. \( \square \)

3.4 Examples

Given crystal lattice \( G \) with the quotient graph \( G^{(\alpha)} \), we assume that the lattice \( L \) is embedded in \( \mathbb{R}^d \). The \( r \)-unit vectors \( \hat{\theta}_1, \ldots, \hat{\theta}_r \in \mathbb{R}^d \) with \( r \geq d \) corresponds to 1-form \( \theta(e_1), \ldots, \theta(e_r) \), \( (e_j \in E^{(\alpha)} \setminus E(T^{(\alpha)})) \); that is, \( \theta(e_j) = \langle \hat{\theta}_j, k \rangle \) for fixed \( k = T(k_1, \ldots, k_d) \in K^d \).

Here \( r = |E^{(\alpha)}| - |E(T^{(\alpha)})| \). From \( \{\hat{\theta}_1, \ldots, \hat{\theta}_r\} \), we can choose \( d \)-linearly independent vectors \( \{\hat{\theta}_1, \ldots, \hat{\theta}_d\} \). Define \( d \times d \) matrix \( J \) by \( J = T[\hat{\theta}_1, \ldots, \hat{\theta}_d] \). The linearly independence implies \( \det(J) \neq 0 \). Taking \( \theta_j \equiv \theta(e_{n_j}) \), remark that \( \partial \phi/\partial k_1 = \partial \phi/\partial k_2 = \cdots = \partial \phi/\partial k_d = 0 \).
if and only if $\frac{\partial \phi}{\partial \theta_1} = \frac{\partial \phi}{\partial \theta_2} = \cdots = \frac{\partial \phi}{\partial \theta_d} = 0$. Moreover since $J \tilde{H}_\theta^T J = H_k$, it is hold that

$$\det(H_k) = \det^2(J) \det(\tilde{H}_\theta).$$

Here

$$(H_k)_{l,m} = \frac{\partial^2 \phi}{\partial k_l \partial k_m} \quad \text{and} \quad (\tilde{H}_\theta)_{l,m} = \frac{\partial^2 \phi}{\partial \theta_l \partial \theta_m}.$$ 

So we use parameters $\theta_1, \ldots, \theta_d$ instead of $k_1, \ldots, k_d$ in the following two examples, triangular lattice and hexagonal lattice. (We treat $\mathbb{Z}^d$ in Sect. 4. more explicitly.) From now on, we confirm that the Grover walks on triangular lattice and hexagonal lattice satisfy assumption (a) and (b). So these walks exhibit both localization and linear spreading.

Figure 2: The quotient graphs of $\mathbb{Z}^d$, triangular lattice and hexagonal lattice

3.4.1 Triangular lattice.

Consider the quotient graph $G^{(o)}$; one vertex with three self loops $\{e_1, e_2, e_3\}$. The 1-form is $\theta(e_1) = \theta_1$, $\theta(e_2) = \theta_2$ and $\theta(e_3) = \theta_3$. It is known that the abelian covering graph of $G^{(o)}$ under the relation $\theta_1 + \theta_2 + \theta_3 = 0$ is the triangular lattice. The transition matrix for the twisted walk on the quotient graph is described by

$$\tilde{P}_k^{(o)} = \frac{1}{3} (\cos \theta_1 + \cos \theta_2 + \cos(\theta_1 + \theta_2)).$$

The critical points are obtained by computing

$$\frac{\partial \phi}{\partial \theta_1} = \frac{\sin \theta_1 + \sin(\theta_1 + \theta_2)}{3 \sin \phi} = 0,$$

$$\frac{\partial \phi}{\partial \theta_2} = \frac{\sin \theta_2 + \sin(\theta_1 + \theta_2)}{3 \sin \phi} = 0,$$

which implies

$$\mathcal{S}_{\phi} = \{(0, \pi), (\pi, 0), (\pm 2\pi/3, \pm 2\pi/3), (\pi, \pi)\}.$$ 

Remark that both numerators and denominators of $\frac{\partial \phi}{\partial \theta_1}$ and $\frac{\partial \phi}{\partial \theta_2}$ at the origin $(\theta_1, \theta_2) = (0, 0)$ are zero. From now on, $(\theta_1, \theta_2) = (0, 0)$ is outside of $\mathcal{S}_{\phi}$. We consider this situation by taking limit of close to the origin using one-parameter $\epsilon \in \mathbb{R}$ in the following setting;
\( \theta_1 = \theta_1(\epsilon) \) and \( \theta_2 = \theta_2(\epsilon) \) with \( \lim_{\epsilon \to 0} \theta_j(\epsilon) = 0 \). Using asymptotics of \( \cos \theta_j(\epsilon) \) and \( \sin \theta_j(\epsilon) \) for small \( \epsilon \); that is, \( \cos \theta_j \sim 1 - \frac{\theta_j^2}{2} \) and \( \sin \theta_j \sim \theta_j \), we have
\[
\frac{\partial \phi}{\partial \theta_1} \sim \frac{\alpha(\epsilon) + 2}{\sqrt{6(\alpha^2(\epsilon) + \alpha(\epsilon) + 1)}}, \\
\frac{\partial \phi}{\partial \theta_2} \sim \frac{2\alpha(\epsilon) + 1}{\sqrt{6(\alpha^2(\epsilon) + \alpha(\epsilon) + 1)}}.
\] (3.59) \hspace{1cm} (3.60)
Here \( \alpha(\epsilon) = \frac{\theta_2(\epsilon)}{\theta_1(\epsilon)} \). We put
\[
x = \frac{t + 2}{\sqrt{6(t^2 + t + 1)}}, \quad y = \frac{2t + 1}{\sqrt{6(t^2 + t + 1)}},
\]
and rotate it a quarter turn
\[
x' = \frac{1}{\sqrt{2}}(x + y), \quad y' = \frac{1}{\sqrt{2}}(-x + y).
\]
Then we have the following equation of ellipse:
\[
(x')^2 + \frac{(y')^2}{\frac{1}{4}} = 1.
\]
It is hold that
\[
(0, 0) \notin \left\{ \left( \frac{t + 2}{\sqrt{6(t^2 + t + 1)}}, \frac{2t + 1}{\sqrt{6(t^2 + t + 1)}} \right) : t \in \mathbb{R} \right\}.
\]
Therefore \( (0, 0) \) is outside of \( S_\phi \).

The Hessian is
\[
H_\theta|_{S_\phi} = \frac{1}{\sin \phi} \left[ \begin{array}{cc} \cos \theta_1 + \cos(\theta_1 + \theta_2) & \cos(\theta_1 + \theta_2) \\ \cos(\theta_1 + \theta_2) & \cos(\theta_1 + \theta_2) + \cos \theta_2 \end{array} \right].
\]
Then we can easily check that for all \( p \in S_\phi \), \( \det(H_\theta(p)) \neq 0 \).

### 3.4.2 Hexagonal lattice.

The hexagonal lattice is the maximal abelian covering graph of \( G^{(o)} = (V^{(o)}, D^{(o)}) \) with
\[
V^{(o)} = \{ u, v \}, \quad D^{(o)} = \{ e_0, e_1, e_2, \bar{e}_0, \bar{e}_1, \bar{e}_2 \},
\]
where \( u = o(e_0) = o(e_1) = o(e_2) \) and \( v = t(e_0) = t(e_1) = t(e_2) \). The 1-form assigns \( \theta(e_0) = 0 \), \( \theta(e_1) = \theta_1 \) and \( \theta(e_2) = \theta_2 \). The transition matrix for the twisted walk on the quotient graph is described by
\[
\tilde{P}_k^{(o)} = \frac{1}{3} \left[ \begin{array}{ccc} 0 & 1 + e^{-i\theta_1} + e^{-i\theta_2} \\ 1 + e^{i\theta_1} + e^{i\theta_2} & 0 \end{array} \right].
\]
Its eigenvalues are \( \{ \pm |1 + e^{i\theta_1} + e^{i\theta_2}|/3 \} \). Taking \( \cos \phi = |1 + e^{i\theta_1} + e^{i\theta_2}|/3 \), we have

\[
\frac{\partial \phi}{\partial \theta_1} = \frac{2 \sin \theta_1 + \sin(\theta_1 - \theta_2)}{9 \sin 2\phi}, \quad (3.61)
\]

\[
\frac{\partial \phi}{\partial \theta_2} = \frac{2 \sin \theta_2 + \sin(\theta_2 - \theta_1)}{9 \sin 2\phi}. \quad (3.62)
\]

The candidates of the critical points are

\[
\{(0, 0), (\pm 2\pi/3, \mp 2\pi/3), (\pm \pi, \mp \pi), (0, \pm \pi), (\pm \pi, \pm \pi)\}
\]

because they are the all solutions for both of the numerators of RHSs in Eqs. (3.61) and (3.62) equal to zero. In the following, we show that the first two candidates \((0, 0)\) and \((\pm 2\pi/3, \mp 2\pi/3)\) are excluded from the critical points. We take also \(\theta_j(\epsilon) = \theta_j(\epsilon) + \alpha(\epsilon) \theta_2(\epsilon)/\theta_1(\epsilon)\).

(1) \((0, 0)\) case: We can evaluate \(\sin \theta_j \sim \theta_j(\epsilon)\) and \(\sin(\theta_1 - \theta_2) \sim \theta_1(\epsilon) - \theta_2(\epsilon),\) moreover

\[
\cos 2\phi = 2 \cos^2 \phi - 1 = -\frac{1}{3} + \frac{4}{9} \left( \cos \theta_1 + \cos \theta_2 + \cos(\theta_1 - \theta_2) \right)\quad (3.63)
\]

\[
\sim 1 - \frac{4}{9} \left( \theta_1^2(\epsilon) + \theta_2^2(\epsilon) - \theta_1(\epsilon) \theta_2(\epsilon) \right). \quad (3.64)
\]

\[
\sin^2 2\phi \sim \frac{8}{9} \left( \theta_1^2(\epsilon) + \theta_2^2(\epsilon) - \theta_1(\epsilon) \theta_2(\epsilon) \right). \quad (3.65)
\]

Inserting these estimations into Eqs. (3.61) and (3.62),

\[
\frac{\partial \phi}{\partial \theta_1} = \frac{2 - \alpha(\epsilon)}{3\sqrt{2}\sqrt{\alpha^2(\epsilon) - \alpha(\epsilon) + 1}}, \quad (3.66)
\]

\[
\frac{\partial \phi}{\partial \theta_2} = \frac{-1 + 2\alpha(\epsilon)}{3\sqrt{2}\sqrt{\alpha^2(\epsilon) - \alpha(\epsilon) + 1}}. \quad (3.67)
\]

We put

\[
x = \frac{2 - t}{3\sqrt{2}\sqrt{t^2 - t + 1}}, \quad y = \frac{-1 + 2t}{3\sqrt{2}\sqrt{t^2 - t + 1}},
\]

and rotate it a quarter turn

\[
x' = \frac{1}{\sqrt{2}}(x + y), \quad y' = \frac{1}{\sqrt{2}}(-x + y).
\]

Then we have the following equation of ellipse:

\[
\frac{(x')^2}{\left(\frac{2}{3}\right)} + \frac{(y')^2}{\left(\frac{1}{3}\right)} = 1.
\]

It is hold that

\[
(0, 0) \notin \left\{ \left( \frac{2 - t}{3\sqrt{2}\sqrt{t^2 - t + 1}}, \frac{-1 + 2t}{3\sqrt{2}\sqrt{t^2 - t + 1}} \right) : t \in \mathbb{R} \right\}.
\]

Therefore \((0, 0)\) is outside of \(S_\phi\).
(2) \((\pm 2\pi/3, \mp 2\pi/3)\) case: We consider \((2\pi/3, -2\pi/3)\) case. Set \(\theta_1 = 2\pi/3 + \eta_1(\epsilon), \theta_2 = -2\pi/3 + \eta_2(\epsilon)\) with \(\eta_j(\epsilon) \to 0\). We estimate

\[
\sin \theta_j \sim \frac{\sqrt{3}}{2} - \frac{1}{2} \eta_j(\epsilon)
\]

\[
|\sin 2\phi| \sim \frac{2}{3} \sqrt{\eta_1^2(\epsilon) + \eta_2^2(\epsilon) - \eta_1(\epsilon)\eta_2(\epsilon)}
\]

Inserting these estimations into Eqs. (3.61) and (3.62),

\[
\frac{\partial \phi}{\partial \theta_1} = \frac{2 - \beta(\epsilon)}{6\sqrt{\beta^2(\epsilon) - \beta(\epsilon) + 1}}, \quad (3.68)
\]

\[
\frac{\partial \phi}{\partial \theta_2} = \frac{2\beta(\epsilon) - 1}{6\sqrt{\alpha^2(\epsilon) - \alpha(\epsilon) + 1}}, \quad (3.69)
\]

We put

\[
x = \frac{2 - t}{6\sqrt{t^2 - t + 1}}, \quad y = \frac{-1 + 2t}{6\sqrt{t^2 - t + 1}},
\]

and rotate it a quarter turn

\[
x' = \frac{1}{\sqrt{2}}(x + y), \quad y' = \frac{1}{\sqrt{2}}(-x + y).
\]

Then we have the following equation of ellipse:

\[
\frac{(x')^2}{\left(\frac{18}{13}\right)} + \frac{(y')^2}{\left(\frac{2}{3}\right)} = 1.
\]

It is hold that

\[
(0, 0) \notin \left\{ \left( \frac{2 - t}{3\sqrt{2}t^2 - t + 1}, \frac{-1 + 2t}{3\sqrt{2}t^2 - t + 1} \right) : t \in \mathbb{R} \right\}.
\]

Therefore \((0, 0)\) is outside of \(S_{\phi}\).

The Hessian is

\[
H_{\theta} |_{S_{\phi}} = \frac{1}{\sin 2\phi} \begin{bmatrix}
\cos \theta_1 + \cos(\theta_1 - \theta_2) & -\cos(\theta_1 - \theta_2)
\-\cos(\theta_1 - \theta_2) & \cos(\theta_1 - \theta_2) + \cos \theta_2
\end{bmatrix}
\]

Then we can easily check that for all \(p \in S_{\phi}, \det(H_{\theta}(p)) \neq 0\).

4 Grover walk on \(\mathbb{Z}^d\) lattice

It is well known that the \(d\)-dimensional square lattice is the maximal abelian covering graph of the \(d\)-bouquet; that is, one vertex with \(d\) self loops \(\{e_1, \ldots, e_d\}\). The 1-form assigns
\( \theta(e_1) = \theta_1, \ldots, \theta(e_d) = \theta_d \). At first, from now on we check the Grover walk on \( \mathbb{Z}^d \) satisfy assumption (1) and (2). We can easily compute that \( \cos \phi = 1/d \cdot \sum_{j=1}^d \cos \theta_j \) which implies

\[
\frac{\partial \phi}{\partial \theta_j} = \frac{\sin \theta_j}{d \sin \phi}.
\] (4.70)

Then all the candidates of the critical points, in which the numerators of RHS in Eq. (4.70) are zero for all \( j \), are as follows:

\[ \{(n_1\pi, \ldots, n_d\pi) : n_j \in \{0,1\}\}. \]

We have to pay attention to \( \{(0, \ldots, 0), (\pi, \ldots, \pi)\} \) case because both numerator and denominator of RHS in Eq. (4.70) at these points are zero. So we take \( \theta_1 = \theta_j(\epsilon) \) with \( \lim_{\epsilon \to 0} \theta_j(\epsilon) = 0 \). We have \( \cos \theta \sim 1 - 1/2 \cdot \theta_j^2(\epsilon) \) and \( \sin \phi \sim \sqrt{K_2(\epsilon)/d} \), where \( K_2(\epsilon) = \sum_{j=1}^d \theta_j^2 \). Inserting these approximations into Eq. (4.70), it is hold that

\[
\frac{\partial \phi}{\partial \theta_j} \sim \frac{1}{\sqrt{d}} \theta_j(\epsilon).
\] (4.71)

Putting \( t_j = \lim_{\epsilon \to 0} \theta_j(\epsilon)/\sqrt{K_2(\epsilon)} \), Eq. (4.71) implies

\[
(t_1, \ldots, t_d) \in \partial B_d,
\]

where \( \partial B_d = \{ \mathbf{x} \in \mathbb{R}^d : ||\mathbf{x}||^2 = 1/d \} \). Obviously \( (0,0) \notin \partial B_d \), then \( (0,0) \) is outside of \( S_\phi \).

In the same way, we obtain \( (\pi, \ldots, \pi) \notin S_\phi \). Thus we have

\[ S_\phi = \{(n_1\pi, \ldots, n_d\pi) : n_j \in \{0,1\}\} \setminus \{(0, \ldots, 0), (\pi, \ldots, \pi)\}. \]

The Hessian is given by Eq. (4.79). For \( \mathbf{p} = (k_1, \ldots, k_d) \in S_\phi \), \( \cos \phi(\mathbf{p}) = 1 - 2m/d \), where \( m \) is number of \(-1\) in the sequence of \( (k_1, \ldots, k_d) \). Then we can easily check that for all \( \mathbf{p} \in S_\phi \),

\[ |\det(H(\mathbf{p}))| = \frac{1}{(d-2m)^d} \neq 0. \]

### 4.1 Localization

As a standard way, we put for \( \hat{\theta}_j \in \mathbb{R}^d \),

\[ \hat{\theta}_1 = T[1,0, \ldots, 0], \hat{\theta}_2 = T[0,1, \ldots, 0], \ldots, \hat{\theta}_d = T[0,0, \ldots, 1]. \]

Since \( |V^{(o)}| = |\{u_l\}| = 1 \), we denote \( \hat{\Psi}_n(\mathbf{x}, u) = \hat{\Psi}_n(\mathbf{x}) \) for \( \mathbf{x} \in \mathbb{Z}^d \) and \( \hat{\Psi}_n(\mathbf{k}, u) = \hat{\Psi}_n(\mathbf{k}) \) for \( \mathbf{k} \in \mathbb{R}^d \). Equation (3.42) implies

\[ \hat{\Psi}_n(\mathbf{k}) = \hat{U}^{(o)}(\mathbf{k})^n \hat{\Psi}_0(\mathbf{k}). \]

Here \( \hat{U}^{(o)}(\mathbf{k}) = \hat{S}^{(o)}(\mathbf{k})G_d \), where \( G_d \) is the \( d \)-dimensional Grover matrix and for \( \mathbf{k} = (k_1, k_2, \ldots, k_d), l \in \{\pm 1, \pm 2, \ldots, \pm d\}, \hat{S}^{(o)}(\mathbf{k})\delta_{\mathbf{e}_l} = e^{ik_l}\delta_{\mathbf{e}_l}. \)
Corollary 2. For the Grover walk on $d$-dimensional lattice, we have

$$\text{spec}(\tilde{U}^{(o)}(k)) = \left\{ e^{\pm i\phi(k)} : \cos \phi(k) = \frac{1}{d} \sum_{j=1}^{d} \cos k_j \right\} \cup \{1\}^{M_1} \cup \{-1\}^{M-1} \quad (4.72)$$

where $M_1 = 1_{\{k=(0,\ldots,0)\}}(k) + (d-1)$, $M-1 = 1_{\{k=(\pi,\ldots,\pi)\}}(k) + (d-1)$. Moreover

1. The normalized eigenvector $v_\phi = T[v_\phi(e_1), v_\phi(\bar{e}_1), \ldots, v_\phi(e_d), v_\phi(\bar{e}_d)]$ for eigenvalue $e^{i\phi}$ with $\phi \notin \{0, \pi\}$ is

$$v_\phi(e_j) = \frac{1}{\sqrt{4d} \sin \phi} \left( 1 - e^{i(\phi-k_j)} \right), \quad v_\phi(\bar{e}_j) = \frac{1}{\sqrt{4d} \sin \phi} \left( 1 - e^{i(\phi+k_j)} \right), \quad (j \in \{1, \ldots, d\}).$$

2. The eigenspace of the eigenvalues $\pm 1$ is expressed by

$$\tilde{L}^{(o)}_k \perp = \text{span}\{u, \tilde{S}^{(o)}(k)u\} \perp.$$

Here $u$ is the uniform vector.

Proof. The characteristic function of the simple random walk $Y_n$ on $\mathbb{Z}^d$ starting from the origin is described by

$$E[e^{i(\phi,Y_n)}] = \left( \frac{\sum_{j=1}^{d} e^{ik_j} + e^{-ik_j}}{2d} \right)^n = \left( \frac{\sum_{j=1}^{d} \cos k_j}{d} \right)^n.$$

Combining it with Proposition 3 leads to the conclusion. \(\square\)

As we see the previous section, $\mathbb{Z}^d$ satisfies the assumptions (a) and (b). Theorem 2 implies the following corollary.

Corollary 3. Let $\gamma$ and $\tau$ be defined in Eqs (2.34) and (2.35), respectively. For $x \in \mathbb{Z}^d$ and $e, f \in D^{(o)}$, Define $c_{x,e,f}$ as the closed path on $\mathbb{Z}^d \times D^{(o)}$ by

$$\left( (x,e), (x+\hat{\theta}(e), f), (x+\hat{\theta}(e) + \hat{\theta}(f), e), (x+\hat{\theta}(f), f) \right).$$

Then we have

$$\mathcal{M}_+ = \sum_{x \in \mathbb{Z}^d, e, f \in D^{(o)}} \mathbb{C} \gamma(c_{x,e,f}), \quad (4.73)$$

$$\mathcal{M}_- = \sum_{x \in \mathbb{Z}^d, e, f \in D^{(o)}} \mathbb{C} \tau(c_{x,e,f}). \quad (4.74)$$

Moreover the time averaged limit measure with the initial state $\Psi_0 \in \mathcal{H}$, $\overline{\mu}_\infty(j) = \lim_{T \to \infty} 1/T \cdot \sum_{n=0}^{T-1} \mu_n(j)$, is expressed by

$$\overline{\mu}_\infty(j) = \left\| \Pi_{\delta_j} \left( \Pi_{\mathcal{M}_+} + \Pi_{\mathcal{M}_-} \right) \Psi_0 \right\|^2. \quad (4.75)$$

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4.2 Weak convergence

In this section, to simplify the problem, the initial state is given by so called mixed state; that is,

\[ P[\Psi_0 = \delta_e] = \frac{1_{\{\langle e \rangle = 0\}}(e)}{2d}. \]

From now on, we consider the weak limit theorems taking the expectation with respect to the initial state. In the mixed state, the statement of Lemma 3 is reduced to the following corollary.

**Corollary 4.** If the initial state is the mixed state, then we have

\[
\lim_{n \to \infty} E[e^{i\langle \xi, X_n \rangle/n}] = \left(1 - \frac{1}{d}\right) + \frac{1}{d} \int_{k \in [0,2\pi)^d} \cos[(\xi, \nabla \phi)] \frac{dk}{(2\pi)^d}.
\]

(4.76)

**Proof.** The first term of RHS in Eq. (3.57) is rewritten by

\[
||\left(\Pi_{\bar{M}+} + \Pi_{\bar{M}-}\right)\tilde{\Psi}_0||^2 = \int_{0,\ldots,d} ||\left(\Pi_{\bar{M}+} + \Pi_{\bar{M}-}\right)\tilde{\Psi}_0||^2 \frac{dk}{(2\pi)^d}.
\]

(4.77)

Because of \( P(\tilde{\Psi}_0 = \delta_{e^n}) = 1/(2d) \), The integrand of RHS in Eq. (4.77) is reduced to

\[
||\left(\Pi_{\bar{M}+} + \Pi_{\bar{M}-}\right)\tilde{\Psi}_0||^2 = \frac{1}{2d} \left(\dim(\bar{M}+) + \dim(\bar{M}-)\right)
\]

\[
= \frac{d-1}{d} \quad (a.s.)
\]

On the other hand, Since

\[
||\Pi_{v_\phi}\tilde{\Psi}_0||^2 = \frac{1}{2d} \text{Tr}[\Pi_{v_\phi}] = \frac{1}{2d},
\]

(4.78)

the integrand of the second term of RHS in Eq. (3.57) is rewritten by

\[
\sum_{\phi} e^{i\langle \xi, \nabla \phi \rangle} ||\Pi_{v_\phi}\tilde{\Psi}_0||^2 = \frac{1}{2d} \left(e^{i\langle \xi, \nabla \phi(k) \rangle} + e^{-i\langle \xi, \nabla \phi(k) \rangle}\right).
\]

We obtain the conclusion. \(\square\)

For \( \phi \in \Phi^{(o)} \setminus \Lambda \) with \( \cos \phi(k) = (\sum_{j=1}^{d} \cos k_j)/d \) and \( \sin \phi(k) > 0 \), we define the Hessian matrix \( \text{Hess}_\phi = (H_d)_{l,m} \) \((l, m \in 1, \ldots, d)\).

**Lemma 4.** Taking \( x_j = \partial \phi(k)/\partial k_j \) with \( \cos \phi(k) = (\sum_{j=1}^{d} \cos k_j)/d \) and \( \sin \phi(k) \geq 0 \), we have

\[
|\det(H_d)| = \prod_{l=1}^{d} \left(\frac{\cos k_l}{d \sin \phi(k)}\right) \left(1 - d \cos \phi(k) \sum_{j=1}^{d} x_j^2 \cos k_j\right).
\]

(4.79)
Proof. Since \( \cos \phi(k) = 1/d \cdot \sum_{j=1}^{d} \cos k_j \), we have

\[
\frac{\partial \phi(k)}{\partial k_m} = \frac{1}{d \sin \phi(k)} \sin k_m.
\] (4.80)

Moreover remarking

\[
x_m = \frac{\partial}{\partial k_m} \phi(k) = \frac{1}{d \sin \phi(k)} \sin k_m,
\] (4.81)

it is obtained that

\[
\frac{\partial}{\partial k_l} \frac{\partial}{\partial k_m} \phi(k) = -\frac{1}{\tan \phi(k)} \left( x_l x_m - \delta_{l,m} \frac{\cos k_l}{d \cos \phi(k)} \right).
\] (4.82)

Thus \( H_d \) is expressed as follows:

\[
H_d = -\frac{1}{\tan \phi(k)} (P - D),
\] (4.83)

where \((P)_{l,m} = x_l x_m\), and \(D = \text{diag}[\cos k_j/(d \cos \phi(k)); 1 \leq j \leq d]\). Now we compute its determinate as follows:

\[
\det(H_d) = \left(-\frac{1}{\tan \phi(k)}\right)^d \det(P - D) = \left(-\frac{1}{\tan \phi(k)}\right)^d \det(D) \det(I - D^{-1}P).
\] (4.84)

Remark that

\[
\det(D) = \prod_{j=1}^{d} \cos k_j \frac{1}{d \cos \phi(k)}
\] (4.86)

\[
\det(I - D^{-1}P) = 1 - \text{Tr}[D^{-1}P]
\] (4.87)

\[
= 1 - \sum_{j=1}^{d} d \cos \phi(k) \frac{\cos k_j}{\cos k_j} x_j^2
\] (4.88)

We used the fact \( \det(I_n - AB) = \det(I_m - BA) \), where \( A \) and \( B \) are \( n \times m \) and \( m \times n \) matrices. Inserting Eqs. (4.86) and (4.88) into Eq. (4.85) completes the proof. \( \square \)

Define the density function of the weak convergence of QW with respect to RHS of the second term in Eq. (3.57) by \( \rho_d(x) \). Replacing \( \partial \phi(k)/\partial k_j \) with \( x_j \) in the integral of RHS in Eq. (3.57), we can find the shape of limit density function \( \rho_d \) from the Hessian matrix \( H_d \), that is, for \( x = (x_1, \ldots, x_d) \),

\[
\rho_d(x) \propto \frac{1}{(2\pi)^d |\det(H_d)|}.
\] (4.89)

**Theorem 4.** For \( d = 2 \),

\[
\rho_2(x, y) = \frac{2 \times 1_{\{x^2+y^2 \leq 1/2\}}(x)}{\pi^2(x+y-1)(x+y+1)(x-y+1)(x-y-1)}.
\] (4.90)
Proof. We can obtain explicit solutions \((k, l) \in K^2\) for
\[
x = \frac{\sin k}{2 \sin \phi (k, l)}, \quad y = \frac{\sin l}{2 \sin \phi (k, l)},
\]
as the function of \(x\) and \(y\):
\[
\cos k = 1 - 3x^2 - y^2 \quad \frac{1}{\sqrt{(x + y - 1)(x + y + 1)(x - y - 1)(x - y + 1)}} \quad (4.91)
\]
\[
\cos l = -1 - 3y^2 - x^2 \quad \frac{1}{\sqrt{(x + y - 1)(x + y + 1)(x - y - 1)(x - y + 1)}} \quad (4.92)
\]
A direct computation of Lemma 4 inserting Eqs. (4.91) and (4.92) leads to the conclusion. \(\square\)

In general \(d \geq 3\), it is hard to directly solve the following system of equations:
\[
x_1 = \frac{\sin k_1}{d \sin \phi (k)}, \quad x_2 = \frac{\sin k_2}{d \sin \phi (k)}, \ldots, \quad x_d = \frac{\sin k_d}{d \sin \phi (k)}.
\]
So it seems to be unfortunately difficult to get a closed expression \(\rho_d\) as a function of \(x \in \mathbb{R}^d\) in the present stage. However in the following, we can partially obtain the shape of \(\rho_d\).

**Theorem 5.** Let the support of \(\rho_d\) be \(S_d \subset \mathbb{R}^d\). Then we have
\[
S_d \subseteq B_d, \quad (4.93)
\]
where \(B_d\) is the \(d\)-dimensional sphere whose radius is \(1/\sqrt{d}\).

Proof.
\[
\sum_{j=1}^{d} x_j^2 = \frac{d}{d \sin \phi (k)} \sum_{j=1}^{d} \left( \frac{1}{d \sin \phi (k)} \right)^2 = \frac{\sum_{j=1}^{d} (1 - \cos^2 k_j)}{d^2} \quad (4.94)
\]
Remark that from the Cauchy-Schwartz inequality,
\[
\left( \sum_{j=1}^{d} \cos k_j \right)^2 \leq d \sum_{j=1}^{d} \cos^2 k_j. \quad (4.95)
\]
Combining Eq. (4.94) with Eq. (4.95), we obtain
\[
\sum_{j=1}^{d} x_j^2 \leq 1/d.
\]
In particular, \(\sum_{j=1}^{d} x_j^2 = 1/d\) if and only if \(c = \cos k_j\) for all \(j \in \{1, \ldots, d\}\). \(\square\)

Put the boundary of \(d\)-dimensional sphere \(B_d\) by \(\partial B_d\). What happens on the boundary of sphere \(B_d\)? The following is the answer:
Theorem 6. Define $V_d$ as the set of vertices for the $d$-dimensional cube inscribed in $B_d$, i.e., $V_d = \{ x = (x_1, \ldots, x_d) \in \mathbb{Z}^d : |x_j| = 1/d \}$. Then

$$
\rho_d(x) = \begin{cases} 
\infty & : x \in V_d, \\
0 & : x \in \partial B_d \setminus V_d \text{ with } d \geq 3, \\
\frac{4}{\pi \cos^2 \frac{\gamma}{2}} & : x \in \partial B_d \setminus V_d \text{ with } d = 2,
\end{cases}
$$

(4.96)

where we put $x = 1/\sqrt{2} \cdot \cos \gamma$ and $y = 1/\sqrt{2} \cdot \sin \gamma$ for $d = 2$ case.

Proof. Let for $k = (k_1, \ldots, k_d)$,

$$
f_j(k) = \frac{1 - \cos^2 k_j}{d^2 - (\cos k_1 + \cdots + \cos k_d)^2} (= x_j^2).
$$

(4.97)

From Eq. (4.95), we have

$$
f_j(k) \leq \frac{1}{d^2}.
$$

(4.98)

Since the equality is hold in the Eq. (4.95) if and only if $x = (x_1, \ldots, x_d) \in \partial B_d$, we focus on the case of the equality is hold in the Eq. (4.82), that is, $c_j \equiv \cos k_j = c$ for some $c \in [-1, 1]$ is hold. Recall that the statement of Lemma 4 is

$$
|\det(H_d)| = \prod_{l=1}^d \left( \frac{\cos k_j}{d \sin \phi(k)} \right) \left( 1 - d \cos \phi(k) \sum_{j=1}^d x_j^2 / \cos k_j \right).
$$

(4.99)

We should require a careful treatment to the $|c| = 1$ case because the product in the RHS becomes infinity.

(1) $|c| < 1$ case:

In this case, $\sin \phi(k) = \sqrt{1 - c^2} \neq 0$ holds. Since $x \in \partial B_d$, $\sum_{j=1}^d x_j^2 = 1/d$. Inserting $\cos k_j = c$ for all $j \in \{1, \ldots, d\}$ into Eq. (4.99), $\det(H_d) = 0$ holds. Moreover also inserting $\cos k_j = c$ for all $j \in \{1, \ldots, d\}$ into Eq. (4.97), we can observe $f_j(k) = x_j^2 = 1/d^2$ which implies $(x_1, \ldots, x_d) \in V_d$. Therefore, from Eq. (4.89), $\rho_d(x)$ takes infinity for $x \in V_d$.

(2) $|c| = 1$ case:

At first we treat $c = 1$ case. We consider the situation by taking a limit of $(k_1, \ldots, k_d) \in \mathbb{R}^d$ to $(0, \ldots, 0)$. To do so, we put $k_j = k_j(\epsilon)$ with $\lim_{\epsilon \to 0} k_j(\epsilon) = 0$, $K_2(\epsilon) = \sum_{j=1}^d k_j^2(\epsilon)$ and $K_4(\epsilon) = \sum_{j=1}^d k_j^4(\epsilon)$.

$$
\cos k_j \sim 1 - \frac{1}{2} k_j^2(\epsilon) \left( 1 - \frac{1}{12} k_j^2(\epsilon) \right), \quad \sin k_j \sim k_j(\epsilon) \left( 1 - \frac{1}{6} k_j^2(\epsilon) \right),
$$

$$
\cos \phi \sim 1 - \frac{K_2(\epsilon)}{2d} \left( 1 - \frac{1}{12} K_2(\epsilon) \right), \quad \sin^2 \phi \sim \frac{K_2(\epsilon)}{d} \left( 1 - \frac{1}{12} K_2(\epsilon) - \frac{1}{4d} K_2(\epsilon) \right)
$$

Here $f(x) \sim g(x)$ means $\lim_{\epsilon \to 0} |f(x)/g(x)| = 1$. Inserting these approximations into Eq. (4.97), we have

$$
x_j^2 \sim \frac{k_j^2(\epsilon)}{d K_2(\epsilon)} \left( 1 - \frac{k_j^2(\epsilon)}{3} + \frac{1}{12} K_4(\epsilon) + \frac{1}{4d} K_2(\epsilon) \right)
$$

(4.100)
Using Eq. (4.100), we have

$$1 - d \cos \phi(k) \sum_{j=1}^{d} \frac{x_j^2}{\cos k_j} \sim -\frac{1}{4} \frac{K_4(\epsilon)}{K_2(\epsilon)} + \frac{1}{4d} \frac{K_2(\epsilon)}{K_2(\epsilon)}$$ \hspace{1cm} (4.101)

On the other hand, it is hold that

$$\prod_{j=1}^{d} c_j \sim \frac{1}{(d K_2(\epsilon))^{d/2}}.$$ \hspace{1cm} (4.102)

Combining Eq. (4.100) with Eqs. (4.101) and (4.102) implies that

$$\det(H_d) \sim \frac{1}{(d K_2(\epsilon))^{d/2}} \left(1 - \frac{d K_4(\epsilon)}{K_2(\epsilon)}\right).$$ \hspace{1cm} (4.103)

From the Cauchy-Schwarz inequality, it is hold that

$$\frac{K_4(\epsilon)}{K_2(\epsilon)} = \frac{\sum_{j=1}^{d} k_j^4(\epsilon)}{\left(\sum_{j=1}^{d} k_j^2(\epsilon)\right)^2} \leq \frac{\sum_{j=1}^{d} k_j^4(\epsilon)}{d \sum_{j=1}^{d} k_j^2(\epsilon)} = \frac{1}{d}.$$ \hspace{1cm} (4.104)

where $\kappa = \lim_{\epsilon \to 0} K_4(\epsilon)/K_2(\epsilon)$. In the same way, for $c = -1$ case, taking $k_j = \pi + k_j(\epsilon)$, we arrive at the same equation as Eq. (4.104) in the limit of $\epsilon \to 0$. For $d = 2$ case, from Eq. (4.100), we can take by using parameter $\gamma \in \mathbb{R}$

$$x_1^2 = \frac{1}{2} \cos^2 \gamma, \quad x_2^2 = \frac{1}{2} \sin^2 \gamma$$

in the limit of $\epsilon \to 0$. Inserting $\kappa = \cos^4 \gamma + \sin^4 \gamma$ into Eq. (4.104),

$$\frac{1}{4 \pi^2} |\det(H_2)|^{-1} = \frac{4}{\pi^2 \cos^2 2\gamma}.$$ \hspace{1cm} (4.104)

Indeed in Eq. (4.90), taking $x = 1/\sqrt{2} \cdot \cos \gamma$, $y = 1/\sqrt{2} \cdot \sin \gamma$, we have

$$\rho_2(x, y) = \frac{4}{\pi^2 \cos^2 2\gamma}.$$ \hspace{1cm} (4.105)

We complete the proof. \hfill \Box
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