

# How does Grover walk recognize the shape of crystal lattice?

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**Abstract** We consider the support of the limit distribution of the Grover walk on crystal lattices with the linear scaling. The orbit of the Grover walk is denoted by the parametric plot of the pseudo-velocity of the Grover walk in the wave space. The region of the orbit is the support of the limit distribution. In this paper, we compute the regions of the orbits for the triangular, hexagonal and kagome lattices. We show

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every outer frame of the support is described by an ellipse. The shape of the ellipse depends only on the realization of the fundamental lattice of the crystal lattice in  $\mathbb{R}^2$ .

**Keywords** Grover walks · Crystal lattice · Limit theorem

## 1 Introduction

The Grover walk is one of the intensively studied mathematical models of quantum walks. These considerable reasons are as follows: (i) the Grover walk is a useful tool in the quantum computing accomplishing so-called quantum speedup (see [1] and its references therein); (ii) there is an underlying random walk which describes a part of the spectrum of the Grover walk [2,3]; (iii) some stochastic behavior of the underlying random walk and also geometric aspects of the graph appear in different forms as the limiting behavior of the induced Grover walk [4,5]; (iv) there is a connection to some graph theoretical and combinatorial aspects inducing inverse problems to classify graphs by some Grover walk's behaviors [6–8]; (v) the Grover walk naturally appears as the potential-free quantum graph [9], which is a system of the Schrödinger equation on the metric graph with the boundary conditions at the vertices preserving the self-adjointness of the Hamiltonian [10].

In this paper, we consider the Grover walk in the context of (iii) restricting the graphs to three typical crystal lattices; triangular, hexagonal and kagome lattices. In particular, we study the orbit of the Grover walker linearly scaled by the large time step  $n$ . The Grover walk on these graphs exhibits both localization and linear spreading [2]. It is known that the orbit is described by the parametric plot of the group velocity in the wave space, and the density corresponding to how frequently the orbit of the Grover walker runs through each small mesh on  $\mathbb{R}^2$  is expressed by the effective mass [11]. We show that the orbit of the Grover walker is included in an ellipse with a rotation (Theorem 4). The shape of the region depends only on the realization of the embedding of the fundamental lattice of the crystal lattice in  $\mathbb{R}^2$ . For the underlying random walk on the crystal lattices, geometric quantities and the realization of the embedding in  $\mathbb{R}^d$  are reflected in the return probability [4,12]. On the other hand, homological structure is reflected as the localization of the induced Grover walk [2,4,13]. However, it has been still an open problem to find geometric properties of the graphs from the behavior of linear spreading of the Grover walk. Although this paper treats the orbits of only special crystal lattices linearly scaled by large time  $n$ , we expect that this is a first step to address to this open problem of the Grover walk and provide an interest of this problem.

This paper is organized as follows. In Sect. 2, the definition of the Grover walk on the connected graph is explained. Section 3 is devoted to a construction of the crystal lattice from the finite graph and an embedding of the crystal lattice in  $\mathbb{R}^2$ . In Sect. 4, we prepare the setting of the Grover walk on the crystal lattice and take a short review on spectral mapping theorem and the limit theorem of this walk. We define the orbit of the Grover walk in this section. In Sect. 5, we give our main theorem for the orbits of the Grover walk on the three crystal lattices and its proof. Finally, we discuss our conjecture of the orbits and verify it by numerical simulations.

### 2 Definition of Grover walk on graph

Let  $G = (V(G), E(G))$  be a graph. We define  $A(G)$  as the symmetric arcs induced by  $E(G)$ . The inverse arc of  $e \in A(G)$  is denoted by  $\bar{e} \in A(G)$ . We denote  $o(e), t(e) \in V(G)$  as the origin and terminal vertices of  $e$ , respectively. If  $G$  is a simple graph, then the arc  $e$  with  $o(e) = u$  and  $t(e) = v$  is denoted by  $(u, v)$ . The cycle  $C$  is the sequence of arcs  $(e_0, \dots, e_{r-1})$  so that  $t(e_j) = o(e_{j+1})$  for every  $j \in \mathbb{Z}/\mathbb{Z}_r$ . The Grover walk on graph  $G$  is defined as follows.

#### Definition 1

- (1) Total Hilbert space:  $\mathcal{H} = \ell^2(A(G)) = \{\psi : A(G) \rightarrow \mathbb{C} \mid \|\psi\|^2 < \infty\}$ . Here the inner product is the standard inner product, that is,  $\langle \psi, \phi \rangle = \sum_{e \in A(G)} \overline{\psi(e)}\phi(e)$ .
- (2) Time evolution:  $U : \mathcal{H} \rightarrow \mathcal{H}$  (unitary) such that

$$(U\psi)(e) = \sum_{f:o(e)=t(f)} \left( \frac{2}{\deg(o(e))} - \delta_{e,\bar{f}} \right) \psi(f).$$

- (3) Finding probability at time  $n$  is defined by  $\mu_n^{(\psi_0)} : V(G) \rightarrow [0, 1]$  with the initial state  $\psi_0 \in \ell^2(A(G))$  ( $\|\psi_0\| = 1$ ) such that

$$\mu_n^{(\psi_0)}(u) = \sum_{e:t(e)=u} |(U^n \psi_0)(e)|^2.$$



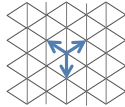


### 3 Crystal lattice and its realization on $\mathbb{R}^d$

Let  $G_0 = (V_0, E_0)$  be a finite graph which may have multi-edges and self-loops. We use the notation  $A_0 := A(G_0)$  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 period lattice  $L$  induced by a subgroup  $H \subset H_1(G_0, \mathbb{Z})$  is denoted by  $H_1(G_0, \mathbb{Z})/H$  [14]. Conceptual figures of  $H_1(G_0, \mathbb{Z})$ ,  $H$  and  $L$  for the base graphs of three-dimensional square lattice, triangular lattice and hexagonal lattice as  $G_0$  are depicted in Fig. 1.

Let the set of basis of  $H_1(G_0, \mathbb{Z})$  be  $\{C_1, C_2, \dots, C_{b_1}\}$  corresponding to fundamental cycles of  $G_0$ , where  $b_1$  is the first Betti number of  $G_0$ . The spanning tree induced by  $\{C_1, C_2, \dots, C_{b_1}\}$  is denoted by  $\mathbb{T}_0$ . The first Betti number  $b_1$  is denoted by  $b_1 = |E_0| - |V_0| + 1$ . A spanning tree of  $G_0$  is a connected subtree of  $G_0$  which covers all the vertices of  $G_0$ . Since the number of edges of the spanning tree is  $|V_0| - 1$ ,  $b_1$  is reexpressed by  $b_1 = |E(G_0)| - |E(\mathbb{T}_0)| = |E(\mathbb{T}_0)^c|$ . Here for a subset  $\Omega'$  of  $\Omega$ ,  $\Omega'^c$  is the complement of  $\Omega'$ , that is,  $\Omega'^c = \Omega \setminus \Omega'$ . Thus, we can take a one-to-one correspondence between  $\{C_1, C_2, \dots, C_{b_1}\}$  and  $E(\mathbb{T}_0)^c$ ; remarking that  $|A(\mathbb{T}_0)| = 2|E(\mathbb{T}_0)|$ , we describe  $C(e) \in \{C_1, C_2, \dots, C_{b_1}\}$  as the fundamental cycle corresponding to  $e \in A(\mathbb{T}_0)^c$  so that  $C(e)$  is the cycle generated by adding  $e \in A(\mathbb{T}_0)^c$  to  $\mathbb{T}_0$ . Set  $\phi : A_0 \rightarrow \mathbb{R}^d$  so that

- (1) for every  $e \in A_0$ ,

$$\phi(\bar{e}) = -\phi(e);$$

$G_0$	$H_1(G_0, \mathbb{Z})$	$H$	$H_1/H$
	$\text{span} \{C_1, C_2, C_3\}$	—	Three-dim square lattice
	$\text{span} \{C_1, C_2, C_3\}$	$C_1 + C_2 + C_3$	
	$\text{span} \{C_1, C_2\}$	—	

**Fig. 1** Examples of  $H_1(G_0, \mathbb{Z})$ ,  $H$  and induced  $L$  for the base graphs of three-dimensional square lattice, triangular lattice and hexagonal lattice cases. The three-dimensional square lattice and the hexagonal lattice are maximal topological crystals, while the triangular lattice is the topological crystal over the three-bouquet graph obtained by the vanishing subgroup  $H = \mathbb{Z}(C_1 + C_2 + C_3)$

(2)

$$\text{rank}[\phi(C_1), \dots, \phi(C_{b_1})] = d.$$

Here for a fundamental cycle  $C_j = (e_0, \dots, e_{r-1})(j \in \{1, \dots, b_1\})$ , we define

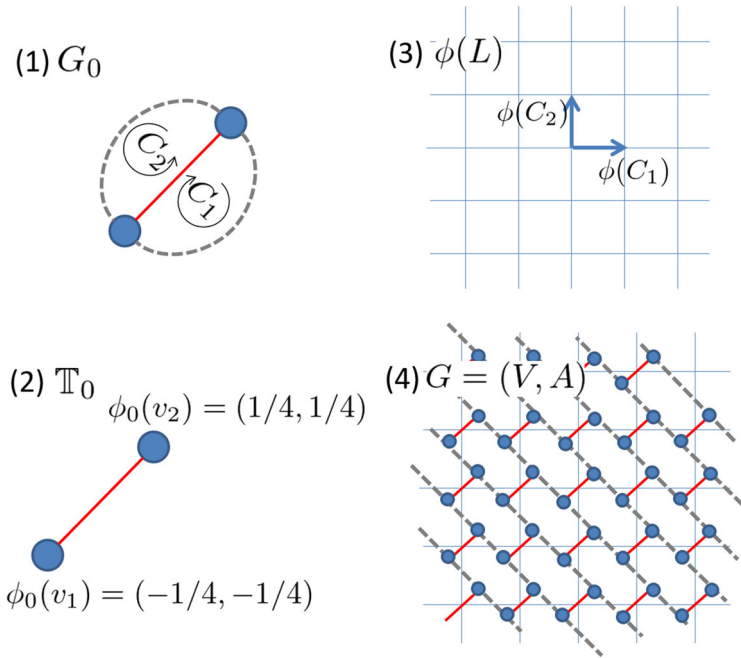
$$\phi(C_j) = \phi(e_0) + \dots + \phi(e_{r-1}).$$

We also set  $\phi_0 : V_0 \rightarrow \mathbb{R}^d$  so that

$$\phi(e) = \phi_0(t(e)) - \phi_0(o(e))$$

for every  $e \in A(\mathbb{T}_0)$ . Thus, the relative coordinate of each vertex of  $G_0$  is determined by  $\phi_0$ . Remark that for every  $e \in A(\mathbb{T}_0)^c$  corresponding to the fundamental cycle  $C = (e_1, \dots, e_r, e)$ ,

$$\phi(e) = \phi(C) + \{\phi_0(o(e_1)) - \phi_0(t(e_r))\} = \phi(C) + \{\phi_0(t(e)) - \phi_0(o(e))\}.$$



**Fig. 2** A realization of the hexagonal lattice. (1)  $G_0$  and basis of homology group. (2) A spanning tree  $\mathbb{T}_0$  of  $G_0$ , and a relative coordinate of each vertex; as an example, we put  $\phi_0(v_1) = (-1/4, -1/4)$ ,  $\phi_0(v_2) = (1/4, 1/4) \in \mathbb{R}^2$ . (3) A realization of the period lattice  $\phi(L)$ ; as an example, we put  $\phi(C_1) = (1, 0)$ ,  $\phi(C_2) = (0, 1) \in \mathbb{R}^2$ . (4) The realization of the covering graph under the setting of (1)–(3); solid edges correspond to the spanning tree of  $G_0$  and dotted edges correspond to  $E(\mathbb{T}_0)^c$

The covering graph  $G = (V, A)$  of  $G_0$  by the abstract period lattice  $L$  is expressed as follows, where  $A$  is the set of the symmetric arcs:

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

See Fig. 2, for a realization of hexagonal lattice.

### 4 Grover walk on the crystal lattice

Let  $\hat{\theta} : A_0 \rightarrow \mathbb{R}^d$  be

$$\hat{\theta}(e) = \begin{cases} \phi(C(e)) & : e \in A(\mathbb{T}_0)^c, \\ 0 & : e \in A(\mathbb{T}_0). \end{cases}$$

It holds  $\hat{\theta}(\bar{e}) = -\hat{\theta}(e)$ . We choose  $e_{i_1}, \dots, e_{i_d}$  from  $A(\mathbb{T})^c$  so that  $\hat{\theta}_1 := \hat{\theta}(e_{i_1}), \dots, \hat{\theta}_d := \hat{\theta}(e_{i_d})$  span  $\mathbb{R}^d$ . We put the following  $d \times d$  matrix by

$$\Theta := {}^t([\hat{\theta}_1, \dots, \hat{\theta}_d]^{-1}).$$

### 4.1 Vertex-based operator: twisted isotropic random walk

Set the Hilbert space generated by  $V = V(G)$  as  $\ell^2(V)$ . Recall that each vertex is represented by some  $x \in L$  and  $u \in V_0$  with  $x + \phi_0(u)$ . We shortly express  $f(x + \phi_0(u))$  by  $f(x; u)$ . We define the Fourier transform with  $k \in [0, 2\pi)^d := \mathcal{T}^d$  by

$$\hat{f}(k; u) = \sum_{x \in L} f(x; u) e^{i\langle \Theta k, x \rangle}.$$

The inverse Fourier transform is expressed by

$$\begin{aligned} f(x; u) &= \int_{\mathcal{T}^d} \hat{f}(k; u) e^{-i\langle \Theta k, x \rangle} \frac{dk}{(2\pi)^d}, \\ &= \frac{1}{|\Theta|} \int_{\Theta(\mathcal{T}^d)} \hat{f}(\Theta^{-1}k; u) e^{-i\langle k, x \rangle} \frac{dk}{(2\pi)^d}, \end{aligned}$$

where  $|\Theta| = \det(\Theta)$ . The random walk operator on  $G$  is described by

$$(Pf)(v) = \sum_{e \in A: t(e)=v} p(e) f(o(e)),$$

for every  $v \in V$ , where  $p(e) = 1/\text{deg}(o(e))$ . Putting  $\hat{P}_k : \ell^2(V_0) \rightarrow \ell^2(V_0)$  by

$$(\hat{P}_k f_0)(u) = \sum_{e \in A_0: t(e)=u} p(e) e^{i\langle \Theta k, \hat{\theta}(e) \rangle} f_0(o(e)),$$

we have

$$\begin{aligned} (P^n f)(x; u) &= \int_{\mathcal{T}^d} \hat{P}_k^n \hat{f}(k; u) e^{-i\langle \Theta k, x \rangle} \frac{dk}{(2\pi)^d} \\ &= \frac{1}{|\Theta|} \int_{\Theta(\mathcal{T}^d)} \hat{P}_{\Theta^{-1}k}^n \hat{f}(\Theta^{-1}k; u) e^{-i\langle k, x \rangle} \frac{dk}{(2\pi)^d}. \end{aligned}$$

Here  $\hat{P}_k$  acts on  $\hat{f}(k; \cdot)$  before taking the integration. We call  $\hat{P}_k$  a twisted random walk on the quotient graph  $G_0$ .

### 4.2 Arc-based operator: twisted Grover walk

Set the Hilbert space generated by  $A = A(G)$  as  $\ell^2(A)$ . Each arc is represented by some  $x \in L$  and  $e \in A_0$  with  $(x; e)$ . We define the Fourier transform with  $k \in \mathcal{T}^d$  by

$$\hat{\psi}(k; e) = \sum_{x \in L} \psi(x; e) e^{i(\Theta k, x)}.$$

The inverse Fourier transform is expressed by

$$\begin{aligned} \psi(x; e) &= \int_{\mathcal{T}^d} \hat{\psi}(k; e) e^{-i(\Theta k, x)} \frac{dk}{(2\pi)^d}, \\ &= \frac{1}{|\Theta|} \int_{\Theta(\mathcal{T}^d)} \hat{\psi}(\Theta^{-1}k, u) e^{-i(k, x)} \frac{dk}{(2\pi)^d}, \end{aligned}$$

where  $|\Theta| = \det(\Theta)$ . The Grover walk operator on  $G$  is described by

$$(U\psi)(e) = \sum_{f \in A: o(e)=t(f)} \left( \frac{2}{\deg(o(e))} - \delta_{\bar{e}, f} \right) \psi(f)$$

for every  $e \in A$ . Putting  $\hat{U}_k : \ell^2(A_0) \rightarrow \ell^2(A_0)$  by

$$(\hat{U}_k \psi_0)(e) = \sum_{f \in A_0: t(f)=o(e)} \left( \frac{2}{\deg(o(e))} - \delta_{\bar{e}, f} \right) e^{i(\Theta k, \hat{t}(f))} \psi_0(f),$$

we have

$$\begin{aligned} (U^n \psi)(x; e) &= \int_{\mathcal{T}^d} \hat{U}_k^n \hat{\psi}(k; e) e^{-i(\Theta k, x)} \frac{dk}{(2\pi)^d} \\ &= \frac{1}{|\Theta|} \int_{\Theta(\mathcal{T}^d)} \hat{U}_{\Theta^{-1}k}^n \hat{\psi}(\Theta^{-1}k; e) e^{-i(k, x)} \frac{dk}{(2\pi)^d}. \end{aligned}$$

Here  $\hat{U}_k$  acts on  $\hat{\psi}(k; \cdot)$  before taking the integration. The unitary operator  $\hat{U}_k$  is called a twisted Grover walk operator.

### 4.3 Via limit distribution

A useful method to get the spectrum of  $\hat{U}_k$  is obtained by [2].

**Theorem 1** [2] (Spectral mapping theorem) *Let  $J(z) = (z + z^{-1})/2$  on the unit circle. Then we have*

$$\sigma(\hat{U}_k) \supseteq J^{-1}(\sigma(\hat{P}_k)); \sigma(\hat{U}_k) \setminus J^{-1}(\sigma(\hat{P}_k)) \subseteq \{\pm 1\}.$$

Let  $\mathcal{C} \subset \ell^2(A_0)$  be the eigenspace which is orthogonal to the eigenspace of  $J^{-1}(\sigma(\hat{P}_k))$ . Then

$$\begin{aligned} \dim \ker(1 - \hat{U}_k|_{\mathcal{C}}) &= b_1; \\ \dim \ker(1 + \hat{U}_k|_{\mathcal{C}}) &= \begin{cases} b_1 : & G_0 \text{ is bipartite,} \\ b_1 - 1 : & G_0 \text{ is non-bipartite,} \end{cases} \end{aligned}$$

where  $b_1$  is the first Betti number of  $G_0$ .

Let  $\mu_n^{(\psi_0)} : A \rightarrow [0, 1]$  be the probability measure at the  $n$ th iteration of  $U$  with the initial state  $\psi_0 \in \ell^2(A)$  such that

$$\mu_n^{(\psi_0)}(x; e_0) = |(U^n \psi_0)(x; e_0)|^2.$$

Putting  $e = (x; e_0)$ , we take the Fourier transform of  $\mu_n^{(\psi_0)}(\cdot; e_0)$  for  $\xi \in \mathbb{R}^d$  by

$$\chi_n(\xi; e_0) := \sum_{x \in L} \mu_n^{(\psi_0)}(x; e_0) e^{i\langle \theta_\xi, x \rangle}.$$

We have the following useful formula which connects the Fourier transform of the amplitude  $\hat{\psi}$  and the Fourier transform of the probability  $\chi_n$ .

**Proposition 1** *Let  $\hat{\psi}_n = \hat{U}_k^n \hat{\psi}_0$ . Then we have*

$$\chi_n(\xi; e_0) = \int_{\mathcal{T}^d} \overline{\hat{\psi}_n(k; e_0)} \hat{\psi}_n(k + \xi; e_0) \frac{dk}{(2\pi)^d}.$$

We join  $\{\chi_n(\xi; e_0)\}_{e_0 \in A_0}$  by

$$\chi_n(\xi) := \sum_{e_0 \in A_0} \chi_n(\xi; e_0).$$

This is rewritten by

$$\chi_n(\xi) = \int_{\mathcal{T}^d} \text{Tr}[\hat{U}_{k+\xi}^n \rho_{k,\xi}^{(0)} \hat{U}_k^{-n}] \frac{dk}{(2\pi)^d},$$

where the matrix representation of  $\rho_{k,\xi}^{(0)}$  is  $(\rho_{k,\xi}^{(0)})_{e,f} = \hat{\psi}_0(k + \xi; e) \overline{\hat{\psi}_0(k; f)}$ . As the initial state, we take the mixed state, i.e.,  $\rho_{k,\xi}^{(0)} = I_{|A_0|} / |A_0|$ . We put the characteristic function with this initial state by  $\chi_n^{(o)}$ .

**Theorem 2** [2] *Let the eigenvalues of  $\hat{P}_k$  be  $\{\cos \gamma_j(k)\}_{j=1}^{|V_0|}$  and we assume  $\gamma_j \in C^\infty$ . Then we have*

$$\lim_{n \rightarrow \infty} \chi_n^{(o)}(\xi/n) = \frac{1}{|E_0|} \int_{\mathcal{T}^d} \sum_{j=1}^{|V_0|} \cos(\langle \xi, \nabla \gamma_j(k) \rangle) \frac{dk}{(2\pi)^d} + \frac{2b_1 - \mathbf{1}_B}{2|E_0|}. \quad (1)$$



Here  $\mathbf{1}_B = 1$  if  $G_0$  is non-bipartite,  $\mathbf{1}_B = 0$  if  $G_0$  is bipartite.

The existence of the second term of (1), which is independent of  $\xi$ , means that localization exhibits in this quantum walk. In this paper, we focus on the first term corresponding to the linear spreading of this quantum walk. If  $H_{\gamma_j} = \det[(\partial^2 \gamma_j / \partial k_\ell \partial k_m)_{\ell, m=1}^d] \neq 0$  for almost every  $k \in \mathcal{T}^d$ , then by replacing the variable  $\nabla \gamma_j(k)$  into  $x \in \mathbb{R}^d$  ( $j \in \{1, \dots, |V_0|\}$ ), the first term of RHS for such a  $j$  is expressed by

$$\int_{x \in \mathbb{R}^d} e^{i(\xi, x)} \rho_j(x) dx$$

Here  $\gamma_j(k)$  is decomposed into  $\gamma_{j,1}(k) + \gamma_{j,2}(k) + \dots + \gamma_{j,\kappa}(k)$  so that for each  $\ell$ ,  $\nabla \gamma_{j,\ell}(k)$  is in one-to-one correspondence with  $x$  and  $\rho_j$  is given by  $\rho_j = \sum_{\ell} (|H_{\gamma_j}|^{-1})_{|\nabla \gamma_{j,\ell}(k)=x}$ .

### 5 Orbit of the quantum walk

Let the eigenvalues of the underlying twisted random walk be denoted by  $\{\gamma_j(k)\}_{j=1}^{|V_0|}$  with  $\Theta = I_d$ . We define the orbit of the quantum walk by

$$\Omega = \bigcup_{j=1}^{|V_0|} \Omega_j \subset \mathbb{R}^d,$$

where

$$\Omega_j := \{\nabla \gamma_j(k) \mid k \in \mathcal{T}^d\}.$$

If we take the embedding of  $L$  by  $L = \{n_1 \hat{\theta}_1 + \dots + n_d \hat{\theta}_d \mid n_1, \dots, n_d \in \mathbb{Z}\}$ , then the support of the continuous limit density function of the quantum walk  $\rho_j$  is expressed by using  $d \times d$  basis transformation matrix  $\tilde{\Theta} := [\hat{\theta}_1, \dots, \hat{\theta}_d] = {}^t(\Theta^{-1})$  as

$$\text{supp}(\rho) = \tilde{\Theta}(\Omega).$$

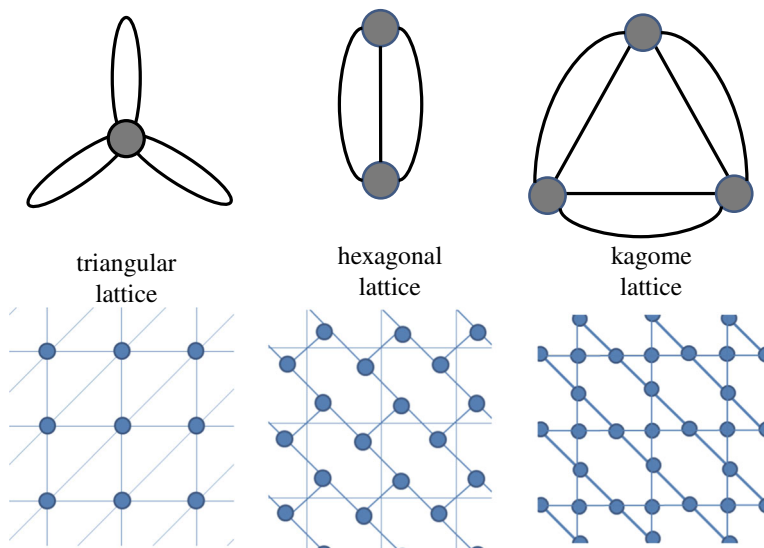
**Theorem 3** [2] *Let  $G$  be the  $d$ -dimensional lattice. Then we have*

$$\Omega \subseteq \{x \in \mathbb{R}^d \mid \|x\|^2 \leq 1/d\}.$$

In this paper, we newly obtain the orbits of the following crystal lattices.

**Theorem 4** *Let  $G \in \{\text{triangular lattice, hexagonal lattice, kagome lattice}\}$  and  $\Omega_G$  be the orbit of Grover walk on  $G$ . Then we have*

$$\Omega_G \subseteq \{(x, y) \in \mathbb{R}^2 \mid x^2 + s(G)xy + y^2 \leq r(G)\}.$$



**Fig. 3** The quotient graphs and realizations with  $\hat{\theta}_1 = {}^t[1, 0], \hat{\theta}_2 = {}^t[0, 1]$

Here

$$r(G) = \begin{cases} 1/2 : & G \text{ is the triangular lattice,} \\ 1/6 : & G \text{ is the hexagonal lattice,} \\ 1/4 : & G \text{ is the kagome lattice,} \end{cases}$$

and

$$s(G) = \begin{cases} -1 : & G \text{ is the triangular lattice,} \\ +1 : & G \text{ is the hexagonal lattice,} \\ +1 : & G \text{ is the kagome lattice.} \end{cases}$$

See Fig. 3 for the realizations of the above graphs on  $\mathbb{R}^2$  in the case of  $\tilde{\Theta} = I_2$ , where  $I_2$  is the two-dimensional identity matrix.

**Corollary 1** *If we embed the above three lattices in  $\mathbb{R}^2$  with the harmonic realization [14] so that each Euclidean length of edge is unit, then*

$$\Omega \subseteq \{x \in \mathbb{R}^2 \mid \|x\|^2 \leq 1/2\}.$$

*Remark 1* The opposite inclusion, that is,

$$\Omega \supseteq \{(x, y) \in \mathbb{R}^2 \mid x^2 + s(G)xy + y^2 \leq r(G)\}$$

is an open problem except the  $G = \mathbb{Z}^2$  case. We discuss it in the final section.

### 5.1 The triangular lattice case

*Proof* The twisted random walk with  $\tilde{\Theta} = I_2$  on the quotient graph of the triangular lattice is

$$\hat{P}_k = \frac{1}{3}(\cos k_1 + \cos k_2 + \cos(k_1 + k_2)).$$

Thus, its spectrum is

$$\sigma(\hat{P}_k) = \frac{1}{3}(\cos k_1 + \cos k_2 + \cos(k_1 + k_2)) = \cos \gamma(k_1, k_2).$$

Then we have

$$x = \frac{\partial \gamma}{\partial k_1} = \frac{\sin k_1 + \sin(k_1 + k_2)}{3 \sin \gamma(k)}, \quad y = \frac{\partial \gamma}{\partial k_2} = \frac{\sin k_2 + \sin(k_1 + k_2)}{3 \sin \gamma(k)}. \tag{2}$$

We take the  $-\pi/4$  rotation as

$$u = \frac{x + y}{\sqrt{2}}, \quad v = \frac{-x + y}{\sqrt{2}}.$$

Thus,

$$u = \frac{\sin k_1 + \sin k_2 + 2 \sin(k_1 + k_2)}{3\sqrt{2} \sin \gamma}, \quad v = \frac{-\sin k_1 + \sin k_2}{3\sqrt{2} \sin \gamma}. \tag{3}$$

Our target is to show

$$\Omega' = \{(u, v) \mid k_1, k_2 \in \mathcal{T}\} = \{(u, v) \in \mathbb{R}^2 \mid u^2 + 3v^2 \leq 1\}.$$

We divide this proof into three steps as follows.

**Lemma 1**

$$\{(u, v) \in \mathbb{R}^2 \mid u^2 + 3v^2 = 1\} \subset \Omega';$$

**Lemma 2**

$$\{(u, v) \in \mathbb{R}^2 \mid u^2 + 3v^2 \leq 1\} \supset \Omega';$$

**Lemma 3**

$$\det(H_\gamma) < \infty$$

for almost every  $k \in \mathcal{T}^2$ .

Since the density of the limit distribution is expressed by the inverse of  $\det(H_\gamma)$ , Lemma 3 means the limit distribution takes positive values for almost every  $(x, y) \in \Omega$ . □

*Proof of Lemma 1* When we take  $(k_1, k_2) = 0$ , then both the numerator and the denominator of  $u$  are 0 and so are those for  $v$ . Then let us consider  $k_1, k_2 \ll 1$ . Using the expansion of  $\sin k_j \sim k_j$  and  $\cos k_j \sim 1 - k_j^2/2$  and taking  $r = k_2/k_1$ , (3) is expressed by

$$u \sim \pm \frac{3 + 3r}{\sqrt{12}\sqrt{1+r+r^2}} := \tilde{u}_\pm(r), \quad v \sim \pm \frac{-1+r}{\sqrt{12}\sqrt{1+r+r^2}} := \tilde{v}_\pm(r). \tag{4}$$

It is easy to check that

$$\tilde{u}_\pm(r)^2 + 3\tilde{v}_\pm(r)^2 = 1.$$

We have

$$\{\tilde{u}_\pm(r) \mid r \in \mathbb{R}\} = [-1, 1], \quad \{\tilde{v}_\pm(r) \mid r \in \mathbb{R}\} = [-1/\sqrt{3}, 1/\sqrt{3}].$$

Then the orbit of  $(\tilde{u}, \tilde{v})$  draws this ellipse, which completes the proof. □

*Proof of Lemma 2* We put  $s_1 = \sin k_1, s_2 = \sin k_2, c_1 = \cos k_1, c_2 = \cos k_2, s_{12} = \sin(k_1 + k_2), c_{12} = \cos(k_1 + k_2)$  and  $c = \cos \gamma, s = \sin \gamma$ . Now our target becomes to show

$$\left(\frac{s_1 + s_2 + 2s_{12}}{3\sqrt{2}s}\right)^2 + 3\left(\frac{-s_1 + s_2}{3\sqrt{2}s}\right)^2 \leq 1 \tag{5}$$

We repeat equivalent transformations of (5) as follows.

$$\begin{aligned} (5) &\Leftrightarrow (s_1 + s_2 + 2s_{12})^2 + 3(-s_1 + s_2)^2 - 18 + 2(c_1 + c_2 + c_{12})^2 \leq 0 \\ &\Leftrightarrow -12 + 2s_1^2 + 2s_2^2 + 2s_{12}^2 - 4s_1s_2 + 4c_1c_2 + 4s_1s_{12} + 4c_1c_{12} + 4s_2s_{12} \\ &\quad + 4c_2c_{12} \leq 0 \\ &\Leftrightarrow -12 + 2(s_1^2 + s_2^2 + s_{12}^2) + 4(c_1c_2 - s_1s_2) + 4(c_1c_{12} + s_1s_{12}) \\ &\quad + 4(c_2c_{12} + s_2s_{12}) \leq 0 \\ &\Leftrightarrow -6 - 2(c_1^2 + c_2^2 + c_{12}^2) + 4(c_{12} + c_1 + c_2) \leq 0 \\ &\Leftrightarrow -2\{(1 - c_1)^2 + (1 - c_2)^2 + (1 - c_{12})^2\} \leq 0 \end{aligned}$$

This completes the proof. □

*Proof of Lemma 3* The determinant of  $H_\gamma$  is expressed by using  $x$  and  $y$  in (2)

$$\det(H_\gamma) = \frac{(c_1 + c_{12} - 3cx^2)(c_2 + c_{12} - 3cy^2) - (c_{12} - 3cxy)^2}{9s^2}.$$

It is obvious that the numerator of RHS is bounded. Thus, only the case for  $s = 0$  has the possibility to provide  $\det(H_\gamma) = \infty$ .

$$\begin{aligned} s = \sin \gamma = 0 &\Leftrightarrow \cos \gamma = \pm 1 \\ &\Leftrightarrow \frac{1}{3}(\cos k_1 + \cos k_2 + \cos(k_1 + k_2)) = \pm 1 \\ &\Leftrightarrow k_1 = k_2 = 0. \end{aligned}$$

Thus, the candidate of the place on  $\mathbb{R}^d$  which produces 0 as the value of the limit density function is on the ellipse. The Lebesgue measure of such a point is zero, which implies the conclusion.  $\square$

### 5.2 The hexagonal graph case

The twisted random walk  $\tilde{\Theta} = I_2$  on the quotient graph of the hexagonal lattice is

$$\hat{P}_k = \begin{bmatrix} 0 & \frac{1}{3}(e^{-ik_1} + e^{-ik_2} + 1) \\ \frac{1}{3}(e^{ik_1} + e^{ik_2} + 1) & 0 \end{bmatrix}.$$

Thus, its spectrum is

$$\sigma(\hat{P}_k) = \pm \frac{1}{3}|1 + e^{ik_1} + e^{ik_2}| = \cos \gamma_{\text{hex}}(k_1, k_2).$$

We put  $\gamma(k_1, k_2) =: \gamma_{\text{hex}}$ . Then we have

$$x = \frac{\partial \gamma_{\text{hex}}}{\partial k_1} = \frac{2 \sin k_1 + \sin(k_1 - k_2)}{9 \sin 2\gamma_{\text{hex}}}, \quad y = \frac{\partial \gamma_{\text{hex}}}{\partial k_2} = \frac{2 \sin k_2 + \sin(k_2 - k_1)}{9 \sin 2\gamma_{\text{hex}}}. \quad (6)$$

We take the  $\pi/4$  rotation as

$$u_{\text{hex}} = \frac{x - y}{\sqrt{2}}, \quad v_{\text{hex}} = \frac{x + y}{\sqrt{2}}.$$

Thus,

$$u_{\text{hex}} = \frac{\sqrt{2} \sin k_1 - \sin k_2 + 2 \sin(k_1 - k_2)}{9 \sin 2\gamma_{\text{hex}}}, \quad v_{\text{hex}} = \frac{\sqrt{2} \sin k_1 + \sin k_2}{9 \sin 2\gamma_{\text{hex}}}. \quad (7)$$

Now our target becomes to show

$$\Omega'_{\text{hex}} = \{(u_{\text{hex}}, v_{\text{hex}}) \mid (k_1, k_2) \in \mathcal{T}\} = \{(u, v) \in \mathbb{R}^2 \mid 3u^2 + 9v^2 \leq 1\}.$$

#### Lemma 4

$$\{(u, v) \in \mathbb{R}^2 \mid 3u^2 + 9v^2 = 1\} \subset \Omega'_{\text{hex}};$$

**Lemma 5**

$$\{(u, v) \in \mathbb{R}^2 \mid 3u^2 + 9v^2 \leq 1\} \supset \Omega'_{\text{hex}};$$

**Lemma 6**

$$\det(H_{\gamma_{\text{hex}}}) < \infty$$

for almost every  $k \in \mathcal{T}^2$ .

*Proof of Lemma 4* When we take  $(k_1, k_2) = 0$ , then both the numerator and the denominator of  $u$  are 0 and also so are those of  $v$ . Then let us consider the case  $k_1, k_2 \ll 1$ . Using the expansion of  $\sin k_j \sim k_j$  and  $\cos k_j \sim 1 - k_j^2/2$  and taking  $r = k_2/k_1$ , (7) is expressed by

$$\begin{aligned} u_{\text{hex}} &\sim \pm \frac{1-r}{2\sqrt{1-r+r^2}} := \tilde{u}_{\pm}(r), \\ v_{\text{hex}} &\sim \pm \frac{1+r}{6\sqrt{1-r+r^2}} := \tilde{v}_{\pm}(r). \end{aligned} \quad (8)$$

It is easy to check that

$$\tilde{u}_{\pm}(r)^2 + 3\tilde{v}_{\pm}(r)^2 = 1/3. \quad (9)$$

We have

$$\{\tilde{u}_{\pm}(r) \mid r \in \mathbb{R}\} = [-1/\sqrt{3}, 1/\sqrt{3}], \quad \{\tilde{v}_{\pm}(r) \mid r \in \mathbb{R}\} = [-1/3, 1/3].$$

Then the orbit of  $(\tilde{u}, \tilde{v})$  draws this ellipse, which completes the proof.  $\square$

*Proof of Lemma 5* We put  $s_1 = \sin k_1, s_2 = \sin k_2, s_{12} = \sin(k_1 - k_2), c_{12} = \cos(k_1 - k_2)$  and  $c = \cos \gamma_{\text{hex}}, s = \sin \gamma_{\text{hex}}$ . Our target is to show

$$3 \left( \frac{\sqrt{2}(s_1 - s_2 + 2s_{12})}{18sc} \right)^2 + 9 \left( \frac{\sqrt{2}(s_1 + s_2)}{18sc} \right)^2 \leq 1. \quad (10)$$

We repeat equivalent transformations of (10) as follows.

$$\begin{aligned} (10) &\Leftrightarrow (s_1 - s_2 + 2s_{12})^2 + 3(s_1 + s_2)^2 \leq 54(sc)^2 \\ &\Leftrightarrow 3(s_1 - s_2 + 2s_{12})^2 + 9(s_1 + s_2)^2 \\ &\quad \leq 4(3 - (c_1 + c_2 + c_{12}))(3 + 2(c_1 + c_2 + c_{12})) \\ &\Leftrightarrow s_1^2 + s_2^2 + s_{12}^2 + (c_1c_2 + c_2c_{12} + c_{12}c_1) - 3 \leq 0 \\ &\Leftrightarrow -(c_1^2 + c_2^2 + c_{12}^2) + \frac{1}{2}((c_1 + c_2 + c_{12})^2 - (c_1^2 + c_2^2 + c_{12}^2)) \leq 0 \\ &\Leftrightarrow (c_1 + c_2 + c_{12})^2 - 3(c_1^2 + c_2^2 + c_{12}^2) \leq 0. \end{aligned}$$

The Cauchy–Schwarz inequality implies the final inequality. It completes the proof.  $\square$

*Proof of Lemma 6* Notice that  $\partial \sin 2\gamma_{\text{hex}}/\partial k_j < \infty$  for  $(j = 1, 2)$  by the above discussion. Therefore, the determinant of  $H_{\gamma_{\text{hex}}}$  is expressed by using a bounded function  $h(k_1, k_2)$  as

$$\det(H_{\gamma_{\text{hex}}}) = \frac{h(k_1, k_2)}{\sin^4 2\gamma_{\text{hex}}}.$$

Only the case for  $\sin 2\gamma_{\text{hex}} = 0$  has a possibility to provide  $\det(H_{\gamma}) = \infty$ . Such points on  $\mathcal{T}^2$  are

$$\{(2\pi/3, -2\pi/3), (-2\pi/3, 2\pi/3), (0, 0)\}.$$

We have already examined the last case  $(0, 0)$ ; the corresponding orbit on  $\mathbb{R}^2$  is the ellipse after the  $\pi/4$  rotation (9). The corresponding first and the second orbits with the  $\pi/4$  rotation on  $\mathcal{R}^2$  are obtained in the same way as the  $(0, 0)$  case: the orbits are obtained by

$$\{(u, v) \mid u^2 + 3v^2 = 1/6\}.$$

Therefore, the places on  $\{(u, v) \in \mathbb{R}^2 \mid u^2 + 3v^2 \leq 1/3\}$  where the value of the density may take zero is described by

$$\{(u, v) \mid u^2 + 3v^2 = 1/6 \text{ or } 1/3\}.$$

The Lebesgue measure of the above set is zero. It completes the proof.  $\square$

### 5.3 The kagome lattice case

The kagome lattice is the line graph of the hexagonal lattice. The transition matrix of the isotropic random walk on a graph  $H$  is denoted by  $P(H)$ . We introduce the following well-known lemma.

**Lemma 7** *Assume  $H$  is a  $\kappa$ -regular graph. Let  $L(H)$  be the line graph of  $H$ . Then we have*

$$\sigma(P(L(H))) = \varphi(\sigma(P(H))) \cup \left\{ \frac{-1}{\kappa - 1} \right\},$$

where  $\varphi(x) = \frac{1}{2(\kappa-1)}(\kappa x + \kappa - 2)$ . Here the dimension of the eigenspace of  $-1/(\kappa - 1)$  is  $|E(H)| - |V(H)|$ .

Thus, the spectrum of the twisted random walk  $\tilde{\Theta} = I_2$  on the kagome lattice is described by

$$\sigma_{0,\text{kag}} := \left\{ \frac{1}{4}(1 \pm |1 + e^{ik_1} + e^{ik_2}|) \right\} \cup \left\{ -\frac{1}{2} \right\} \tag{11}$$

We define  $\cos \gamma_{\text{kag}} := (1/4) + (3/4) \cos \gamma_{\text{hex}} \in \sigma_{0,\text{kag}}$ . Then we have

$$\begin{aligned} \frac{\partial \gamma_{\text{kag}}}{\partial k_1} &= g(k_1, k_2) \frac{\partial \gamma_{\text{hex}}}{\partial k_1}, \\ \frac{\partial \gamma_{\text{kag}}}{\partial k_2} &= g(k_1, k_2) \frac{\partial \gamma_{\text{hex}}}{\partial k_2}, \end{aligned}$$

where

$$g(k_1, k_2) := \frac{3 \sin \gamma_{\text{hex}}}{4 \sin \gamma_{\text{kag}}} = \sqrt{3} \sqrt{\frac{1 + \cos \gamma_{\text{hex}}}{5 + 3 \cos \gamma_{\text{hex}}}}.$$

Taking the  $\pi/4$  rotation, we have

$$u_{\text{kag}} = g(k_1, k_2)u_{\text{hex}}, \quad v_{\text{kag}} = g(k_1, k_2)v_{\text{hex}}. \tag{12}$$

Remark that  $0 \leq g(k_1, k_2) \leq g(0, 0) = \sqrt{3}/2$ . Therefore, using the previous fact on the hexagonal lattice, we have

$$u_{\text{kag}}^2 + 3v_{\text{kag}}^2 \leq 1/4.$$

The equality holds if and only if  $(k_1, k_2) = (0, 0)$ . When  $k_1, k_2 \ll 1$  with  $k_1/k_2 = r$ , then  $g(k_1, k_2) = \sqrt{3}/2 + O(\|(k_1, k_2)\|)$ . Therefore, we have

$$\{(u, v) \mid u^2 + 3v^2 = 1/4\} \subset \Omega'_{\text{kag}} \subset \{(u, v) \mid u^2 + 3v^2 \leq 1/4\}.$$

The determinant of  $H_{\gamma_{\text{kag}}}$  is also expressed by using a bounded function  $s(k_1, k_2)$  as

$$\det(H_{\gamma_{\text{kag}}}) = \frac{s(k_1, k_2)}{(5 + 3 \cos^2 \gamma_{\text{hex}}) \sin^4 2\gamma_{\text{hex}}}.$$

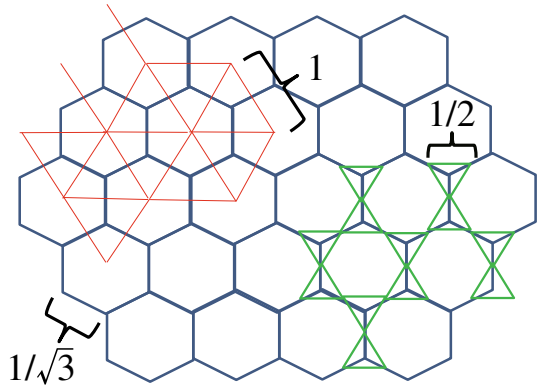
Only the case for  $\sin 2\gamma_{\text{hex}} = 0$  has a possibility of  $\det(H_{\gamma_{\text{kag}}}) = \infty$ . Thus, we can use the argument for the previous hexagonal lattice case. It completes the proof.  $\square$

### 6 Summary and discussion

We obtained the outer frames of the orbits of the Grover walker on some crystal lattices. We have shown that every orbit only depends on the embedding way of the fundamental lattices  $L = \text{span}\{\hat{\theta}_1, \hat{\theta}_2\}$  in  $\mathbb{R}^2$ . If we choose the embedding way so that  $\hat{\theta}_1 = {}^t[1, 0]$ ,  $\hat{\theta}_2 = {}^t[0, 1]$ , the outside frames are described by an ellipse. With the  $\pm\pi/4$  rotations, the orbits are expressed by



**Fig. 4** Triangular and kagome lattices as the dual and line graphs of hexagonal lattice



$$\begin{aligned} \Omega'_{\text{tri}} &\subseteq \{(u, v) \in \mathbb{R}^2 \mid u^2 + 3v^2 \leq r_{\text{tri}}^2\}, \\ \Omega'_{\text{hex}} &\subseteq \{(u, v) \in \mathbb{R}^2 \mid u^2 + 3v^2 \leq r_{\text{hex}}^2\}, \\ \Omega'_{\text{kag}} &\subseteq \{(u, v) \in \mathbb{R}^2 \mid u^2 + 3v^2 \leq r_{\text{kag}}^2\}, \end{aligned}$$

where  $r_{\text{tri}} = 1$ ,  $r_{\text{hex}} = 1/\sqrt{3}$  and  $r_{\text{kag}} = 1/2$ . When we take the harmonic realization to the hexagonal lattice whose Euclid edge length is  $r_{\text{hex}}$  and take dual graph and line graph to this embedding, we obtain triangular lattice and kagome lattice, respectively. The Euclidean edge length of them is  $r_{\text{tri}}$  and  $r_{\text{kag}}$ , respectively; see Fig. 4.

The natural question may arise about the interior. We have the following conjecture.

*Conjecture 1* Let  $G \in \{\text{triangular lattice, hexagonal lattice, kagome lattice}\}$  and  $\Omega_G$  be the orbit of Grover walk on  $G$ . Then we have

$$\Omega_G = \{(x, y) \in \mathbb{R}^2 \mid x^2 + s(G)xy + y^2 \leq r(G)\}.$$

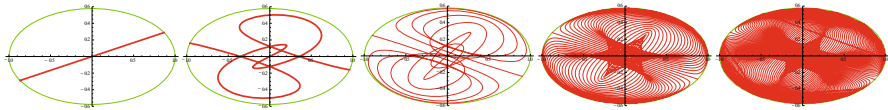
The orbit  $\Omega'_G$  after  $s(G)\pi/4$  rotation is expressed by

$$\Omega'_G = \{(u(k_1, k_2), v(k_1, k_2)) \mid k_1, k_2 \in [0, 2\pi)\},$$

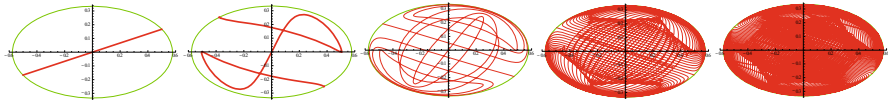
where  $u, v : [0, 2\pi)^2 \rightarrow \mathbb{R}$  are given by (3) for “ $G = \text{triangular lattice}$ ”, (7) for “ $G = \text{hexagonal lattice}$ ”, and (12) for “ $G = \text{kagome lattice}$ ”. Figures 5, 6 and 7 depict the subregions of  $\Omega'_G$  numerically, which is the basis of our conjecture:

$$\Omega_r = \{(u(k, rk), v(k, rk)) \mid k \in [0, 2\pi)\} \subset \Omega'_G$$

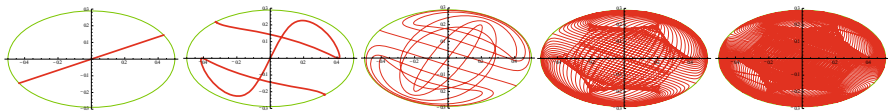
for  $r = 0, 3, 10, 50, 100$  cases. Note that  $r$  corresponds to the pitch winding the torus  $\mathcal{T}^2$ , that is, the larger the pitch  $r$  is, the more places of  $\mathcal{T}^2$  “ $(k, rk)$ ” visits.



**Fig. 5** The orbits of  $\Omega'_r$  for the triangular lattice case by numerical simulation ( $r = 0, 3, 10, 50, 100$ )



**Fig. 6** The orbits of  $\Omega'_r$  for the hexagonal lattice case by numerical simulation ( $r = 0, 3, 10, 50, 100$ )



**Fig. 7** The orbits of  $\Omega'_r$  for the kagome lattice case by numerical simulation ( $r = 0, 3, 10, 50, 100$ )

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