Role of the coin in the spectrum of quantum walks

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Abstract

The most elementary quantum walk is characterized by a 2-dimensional unitary coin flip matrix, which can be parameterized by 4 real variables. The influence of the choice of the coin flip matrix on the time evolution operator is analysed in a systematic way. By changing the coin parameters, the dispersion and asymmetry of eigenvalues of the time evolution operator can be tuned in a controlled way. The reduced eigenvectors in coin space are distributed along trajectories on the surface or inside the Bloch sphere, depending on the degeneracy of the spectrum. At certain values of the coin parameters the spectrum of the time evolution operator becomes 2-fold degenerate, but there might exist unique eigenvalues at the top and bottom of each quasi-energy band. The eigenstates corresponding to such eigenvalues are robust against arbitrary temporal variations in the bias parameter of the coin, as long as rest of the parameters remain unchanged.

1 Introduction

Quantum information and computation is a field which uses concepts from computer science to understand the ability of quantum systems to store and transmit information and to perform computations. The quantum walk is a prime example of this vast field: it was conceived by adopting the concept of random walks from classical information theory to quantum dynamics. The quantum mechanical version of the random walks shows interference effects which might allow faster algorithms than those based on the classical random walks.

Quantum walks have been studied intensively for over a decade. The discrete-time quantum walk was introduced as a unitary process where a single particle, called the walker, hops on a lattice and the direction of movement is decided by its internal state, called the coin degree of freedom [1, 2, 3]. The propagation of the walker is ballistic as opposed to classical random walks where the walker propagates diffusively. The proposition of quantum walks led to studies on whether this effect could be used to design computational algorithms with a quantum speedup [4, 5, 6]. The simplicity of the quantum walk model has also inspired many studies on various aspects of quantum dynamics and quantum information, such as localisation [7, 8], quantum to classical transition [9] and quantum state transfer [10, 11, 12, 13]. Moreover, it has been shown that the quantum walk can be used to perform universal quantum computation [14, 15]. Overviews on the properties of quantum walks can be found in Refs. [16, 17]. They have also been implemented experimentally with optical lattices [18, 19], trapped ions [20, 21] and optical photons [22, 23, 24].

The quantum walks come in many varieties. Ultimately the walks are defined by the underlying lattice structure and the transition rules for moving between the lattice sites. Together they define the time evolution operator, which describes the evolution of the wave function between subsequent time steps. The behaviour of the walk is entirely determined by the eigenvalues and -vectors of the time evolution operator, and the initial state of the walker. The purpose of this paper is to explore the variety of the spectrum of
the time evolution operator with arbitrary 2-dimensional unitary coins for translationally
invariant discrete-time quantum walks on the $N$-cycle. The eigenvalues and eigenvectors
for this problem have been solved by Tregenna et al [25], who also derived formulas for the
asymptotic time-averaged probability distributions in terms of arbitrary coin parameters.
In this paper, we show that by choosing an appropriate parameterization for the coin,
each parameter plays a distinct role in the properties of the eigenvalues and eigenstates.
The solution allows therefore to design quantum walks which have precisely the desired
spectral features. For example, the gaps between the eigenvalues determine important
properties of the walk, such as mixing time [2], and it is desirable to have control over
such features.

To further investigate the properties of the eigenstates, we obtain the Bloch representa-
tion of the reduced eigenvectors in coin space, and study the properties of the eigenvectors
as a function of coin parameters. The eigenvectors are found to be distributed
along well-defined trajectories on the surface or inside the Bloch ball, depending on the
degeneracy of the spectrum. With special attention to degenerate eigenvalues, we point
out that there may also exist unique eigenvalues in an otherwise degenerate spectrum.
The eigenstates corresponding to the unique eigenvalues have very special properties,
since they remain fixed for arbitrary variations of the bias parameter of the coin. These
states are thus protected from arbitrary temporal variations of the bias parameter, if the
rest of the parameters remain fixed.

This article is organized as follows. The discrete-time quantum walk and the param-
eterization of the coin is introduced in Sec. 2. The eigenvalue spectrum is studied in
Sec. 3, and the Bloch representation of the eigenvectors is given in Sec. 4. The protected
eigenstates are discussed in Sec. 5, and the conclusions are presented in Sec. 6.

2 Discrete-time quantum walk

The discrete-time quantum walk proceeds by repeated steps of coin flipping and transla-
tion to the left or right, depending on the state of the coin [1, 2]. The walk is assumed to
take place on a 1-dimensional lattice with periodic boundary conditions, and translation
invariance is imposed by taking the same coin at every site of the lattice. The wave func-
tion of the walker can be written as $|\psi(t)\rangle = \sum_{x,c} \psi_{xc}(t) |x\rangle |c\rangle$, where the amplitudes
$\psi_{xc}(t)$ are complex numbers. The number of sites is $N$ and the coin variable $c$ can take
dependent values $\{0, 1\}$. The total Hilbert space is a tensor product of the spatial and coin spaces,$|\psi(t)\rangle \in \mathbb{H}_X \otimes \mathbb{H}_C$, with dimension $2N$.

The time-independent step operator $U$ evolves the wave function by one time step:
$|\psi(t+1)\rangle = U |\psi(t)\rangle$. It can be written as $U = TF$, where the coin flip acts on the
coin degrees of freedom only: $F = I \otimes F$. The coin flip $F$ is represented by a 2-
dimensional unitary matrix. Such a matrix has generally 8 real components, since each of
the 4 complex elements can be represented by 2 real numbers. Requiring the matrix
to be unitary, $FF^\dagger = F^\dagger F = I$, imposes 4 independent conditions for the elements,
and therefore the matrix is represented by 4 independent real parameters. One of the
parameters is just the total complex phase of the matrix, and it will be ignored since
it does not have any effect on the time evolution of the probability distribution of the
walker. The rest of the parameters can be chosen in infinitely many ways, but as will be
seen below, the following parameterization is particularly insightful when studying the
spectrum of $U$:

$$F = e^{i\beta} \begin{pmatrix}
\sqrt{R} e^{i\alpha} & \sqrt{1-R} e^{-i\beta} \\
-\sqrt{1-R} e^{i\beta} & \sqrt{R} e^{-i\alpha}
\end{pmatrix}$$

(1)
The range of the parameter $R$ is $[0, 1]$ and it is known as the bias parameter, as it sets the
weight between the coin components 0 and 1. The angular variables are on the interval
where the matrix elements are given by 3 components \( \tilde{\psi} \) notation will be useful later.

The conditional shift operator \( T \) moves the walker to the left or right depending on its coin state. It can be written concisely as

\[
T = T_- \otimes P_0 + T_+ \otimes P_1
\]

where the operator \( P_c = |c\rangle \langle c| \) is a projector to the coin state \( c \), and \( T_\pm = \sum_{x \in \mathbb{Z}} |x \pm 1\rangle \langle x| \) is the translation operator. Periodic boundary conditions are imposed by defining the translations at the righthand boundary as \( |N\rangle \langle N-1| = |0\rangle \langle N-1| \) and at the lefthand boundary as \( |-1\rangle \langle 0| = |N-1\rangle \langle 0| \).

### 3 Eigenvalue spectrum

The eigenvalues of the time evolution operator \( U \) can be solved by standard methods of quantum mechanics. Translation invariance implies that the wavenumbers \( k \) in Fourier space are good quantum numbers, which means that the eigenvalue equation for \( U \) becomes \( 2 \times 2 \) block-diagonal, and each block can be solved independently. Since \( U \) is unitary, its eigenvalues are complex numbers with absolute value 1 and can be written as \( e^{i \lambda} \). The phases \( \lambda \) can be interpreted as quasi-energies, if the time evolution of the wave function is thought to be generated by a time-independent Hamiltonian \( H \). The time evolution operator is then given by \( U = e^{-i H \Delta t} \), where the time step is chosen as \( \Delta t = 1 \). Indeed, the quasi-energies \( \lambda \) are distributed along single-particle energy bands that become continuous as the size of the lattice approaches infinity. The eigenvalues and eigenvectors for the \( N \)-cycle with a similar parameterization for the coin have been previously solved by Tregenna et al \[25\], but the solution is summarized here since the notation will be useful later.

The eigenvalue problem for the time evolution operator is given by the equation

\[
U |\psi_\lambda\rangle = e^{i \lambda} |\psi_\lambda\rangle,
\]

where the eigenvectors are denoted by \( |\psi_\lambda\rangle = \sum_{x,c} \tilde{\psi}_\lambda(x, c)|x\rangle|c\rangle = \sum_{k,c} \tilde{\psi}_\lambda(k, c)|k\rangle|c\rangle \) and the Fourier-transformed amplitudes are \( \tilde{\psi}_\lambda(k, c) = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} e^{i 2 \pi k x / N} \psi_\lambda(x, c) \). The task is to find the eigenvalue phases \( \lambda \in [-\pi, \pi) \) and the components of the eigenvectors \( \psi_\lambda \). In the Fourier basis, the translation operators \( T_- \) and \( T_+ \) act diagonally and the wave function is just multiplied by a phase \( e^{-i 2 \pi k / N} \) and \( e^{i 2 \pi k / N} \), respectively. Thus, the \( 2N \) equations in Eq. \[3\] factorize into \( N \) pairs of decoupled equations, involving only the components \( \tilde{\psi}_\lambda(k, 0) \) and \( \tilde{\psi}_\lambda(k, 1) \) at each wavenumber \( k \):

\[
\begin{pmatrix}
00 & 01 \\
01 & 11
\end{pmatrix}
\begin{pmatrix}
\tilde{\psi}_\lambda(k, 0) \\
\tilde{\psi}_\lambda(k, 1)
\end{pmatrix}
= 0
\]

where the matrix elements are given by

\[
\begin{align*}
g_{00}(\lambda, k) &= \sqrt{R} e^{i(\alpha + \beta - 2\pi k / N)} - e^{i \lambda} \\
g_{01}(k) &= -\sqrt{1 - R} e^{i(2\beta + 2\pi k / N)} \\
g_{01}(k) &= \sqrt{1 - R} e^{-i 2\pi k / N} \\
g_{11}(\lambda, k) &= \sqrt{R} e^{-i(\alpha - 2\pi k / N)} - e^{i \lambda}
\end{align*}
\]

for fixed coin parameters \( R, \alpha, \beta \). Denoting the matrix in Eq. \[4\] as \( G \), this equation has non-trivial solutions if and only if the determinant of \( G \) is zero. For most choices of the coin parameters, non-trivial solutions exist for only one wavenumber \( k \), and the
Figure 1: Distribution of the eigenvalue phases $\lambda(k,z)$ as a function of $k$ and $z$. a) Deformation of the spectrum as $R$ varies from 0 to 1. The eigenvalues with the same $R$ are marked with the same colour; the negative (positive) values correspond to $z=1$ ($z=2$). The system size is $N=20$ and the values of the other coin parameters are $\alpha=0$, $\beta=0$. b) Dependence on the coin parameters $\alpha$ and $\beta$. The system size is $N=10$ and $R=0.5$. For the lower bands $z=1$, $\beta=0$, and for the upper bands $z=2$, $\alpha=0$.

eigenvectors are strictly localized at each $k$. There exist however special points in the parameter space where the spectrum becomes degenerate and Eq. (4) allows solutions for two different wavenumbers, as discussed below.

The eigenvalues $e^{i\lambda}$ can be solved from Eq. (4) for each $k$, and there exist two distinct solutions labeled by an integer $z = \{1, 2\}$:

$$e^{i\lambda(k,z)} = e^{i\beta} \left[ \sqrt{R \cos(\alpha - 2\pi k/N)} + i (-1)^z \sqrt{1 - R \cos^2(\alpha - 2\pi k/N)} \right].$$  \hfill (9)

where the term in the square brackets is a complex number with modulus 1. The $2N$ eigenvalues are thus labeled by the wavenumber $k = \{0, 1, \ldots, N-1\}$ and the integer $z$. The eigenvalue phases $\lambda(k,z)$ are plotted as functions of $k$ and $z$ in Fig. 1 for different values of the coin parameters. The eigenvalues for different $k$ are distributed on two well-defined quasi-energy bands, labeled by the integer $z$. The shape of the bands is entirely determined by the coin variables $R$, $\alpha$ and $\beta$, and changing the total number of sites changes only the relative distances of the eigenvalues along the band. As $N \to \infty$, the eigenvalues on each band become infinitesimally close to each other.

Each of the parameters $R$, $\alpha$ and $\beta$ correspond to different properties of the spectrum. As seen in Fig. 1a), the parameter $R$ determines the general shape of the spectrum, interpolating between a completely flat spectrum at $R = 0$ and a linearly spaced spectrum at $R = 1$. In the former case the eigenvalues are $N$-fold degenerate, while in the latter case the gaps between the eigenvalues are degenerate. In the special case $R = 0$, Eq. (9) implies that the phases of the eigenvalues are given by

$$\lambda(k,z) = \beta + (-1)^z \frac{\pi}{2} \forall k; \quad R = 0,$$

and for $R = 1$ they become

$$\lambda(k,z) = \begin{cases} 
\beta + (-1)^z (\alpha - 2\pi k/N) & \text{if } \sin(\alpha - 2\pi k/N) \geq 0 \\
\beta - (-1)^z (\alpha - 2\pi k/N) & \text{if } \sin(\alpha - 2\pi k/N) < 0 
\end{cases} \quad R = 1.$$

Eq. (11) shows clearly that the eigenvalue phases for $R = 1$ are distributed symmetrically around the value $\beta$, with equally spaced intervals $\Delta \lambda = 2\pi/N$.

The role of the parameter $\beta$ is just to set the “base point” of the spectrum, as can be seen directly from Eq. (9). The effect of changing $\beta$ is that each eigenvalue phase is shifted
by a constant amount $\Delta \lambda = \Delta \beta$, as illustrated in Fig. 1b) for the $z = 2$ eigenvalues. The role of the parameter $\alpha$ is slightly more subtle. As shown in Fig. 1b) for the $z = 1$ eigenvalues, increasing the value of $\alpha$ increases $\lambda$ for one half of the spectrum, and decreases $\lambda$ for the other half. Changing the value of $\alpha$ introduces asymmetry between the left and right parts of the spectrum. If the change in $\alpha$ is an integer multiple of $2\pi/N$, this corresponds to a mere relabeling of the wavenumbers $k$, which is evident from Eq. (9). Therefore the spectra corresponding to $\alpha = -\pi/N$ and $\alpha = \pi/N$ in Fig. 1b) are equal, except that the values are shifted horizontally by $\Delta k = 1$.

For most values of $\alpha$, the eigenvalues on the left and right side are not equal, and the spectrum is nondegenerate. Thus, the left-moving and right-moving components of the walker are distinguishable, and the walk is called **chiral**.

### 4 Bloch representation for eigenvectors

In the previous section, it was seen that each coin parameter $R, \alpha, \beta$ has a distinct role in the eigenvalue spectrum of $U$. It turns out that the coin parameters also control different features of the eigenstates. We obtain a geometric picture of the eigenstates which proves to be very useful in the analysis of the eigenstates.

The eigenstates take different forms in the degenerate and non-degenerate cases. The condition that two eigenvalues are equal, $e^{i\lambda(k,z)} = e^{i\lambda(k',z')}$ leads to the following relations:

$$\cos(\alpha - 2\pi k/N) = \cos(\alpha - 2\pi k'/N)$$  \hspace{1cm} (12)

$$(-1)^z \sqrt{1 - R \cos^2(\alpha - 2\pi k/N)} = (-1)^{z'} \sqrt{1 - R \cos^2(\alpha - 2\pi k'/N)}$$  \hspace{1cm} (13)

The second condition is just equal to $z = z'$, since the signs must be equal on both sides. The first condition allows two solutions for the wavenumbers, either $k' = k$ or

$$k' = -k + \frac{N}{\pi} \mod N.$$  \hspace{1cm} (14)

Since the wavenumbers are labeled by integers, the above equation only makes sense if $\alpha$ is an integer multiple of $\pi/N$. Therefore the spectrum becomes degenerate at $2N$ discrete values of $\alpha$:

$$\alpha = n \frac{\pi}{N} \hspace{1cm} n \in \{0, 1, \ldots, 2N-1\}. \hspace{1cm} (15)$$

A similar result has also been obtained by Tregenna et al [25]. In the maximally degenerate case, there are $N$ distinct eigenvalues, which are labeled by $N/2$ pairs of conjugate wavenumbers $(k, k')$ and the integer $z$, and the eigenvalues are labelled by $\lambda(k, k', z)$.

Recall from Eq. (4) that the components of the eigenvectors for wavenumber $k$ can be non-zero iff $\det(G) = g_{00}g_{11} - g_{10}g_{01} = 0$. By a straightforward calculation, it can be shown that this condition is equal to Eq. (12). Therefore, if the spectrum is non-degenerate, only the $k' = k$ component of the eigenvectors is non-zero, and the eigenvectors are localized at wavenumber for each eigenvalue $\lambda(k, z)$. If $\alpha$ is an integer multiple of $\pi/N$, the $k'$-component of the eigenvectors is also non-zero, where the conjugate component $k''$ is given by Eq. (14).

The relations between the two coin components are trivially solved from the first row of Eq. (4):

$$\tilde{\psi}_\lambda(k, 1) = -\frac{g_{00}(\lambda, k)}{g_{01}(k)} \tilde{\psi}_\lambda(k, 0)$$  \hspace{1cm} (16)

$$\tilde{\psi}_\lambda(k', 1) = -\frac{g_{00}(\lambda, k')}{g_{01}(k')} \tilde{\psi}_\lambda(k', 0)$$  \hspace{1cm} (17)

$$\tilde{\psi}_\lambda(k'', c) = 0 \hspace{1cm} \forall c, k'' \neq k, k'.$$  \hspace{1cm} (18)
where |g_{01}| > 0 if R < 1 and \( \lambda = \lambda(k, k', z) \). The condition (17) refers to the non-degenerate case only. The second row of Eq. (4) is then always true if \( \det G = 0 \).

To gain some insight to the properties of the eigenstates, it is useful to move to a geometric picture. The reduced density matrix of the coin, \( \rho_C = \text{Tr}_\chi(\ket{\psi_\lambda}\bra{\psi_\lambda}) \), is a 2 \times 2 matrix that can be represented by a vector \( \vec{r} \), pointing to a point inside the Bloch ball [26]. The density matrix is given by \( \rho_C = \frac{1}{2}(I + \vec{r} \cdot \vec{\sigma}) \), where the \( \sigma_i \) are the Pauli matrices. If the spectrum of \( U \) is non-degenerate, the eigenstates are product states of wavenumbers and coin states, the reduced coin eigenvectors are pure states, and the Bloch vector points always to the surface of the sphere. In the degenerate case, the eigenvectors are not necessarily product states, and the Bloch vector might be inside the sphere. To obtain an explicit representation for the eigenvectors, it is necessary to obtain an orthonormal eigenbasis.

From Eqs. (16–18), the eigenvectors for degenerate eigenvalues can be constructed as

\[
|\psi_\lambda\rangle = s|k\rangle\left[|0\rangle - \frac{g_{00}(\lambda, k)}{g_{01}(k)}|1\rangle\right] + e^{i\omega} s'|k'\rangle\left[|0\rangle - \frac{g_{00}(\lambda, k')}{g_{01}(k')}|1\rangle\right]
\]  

where \( s \) and \( s' \) are real numbers and the complex phase of the \(|k\rangle|0\rangle\)-component is set to 0. The variables \( s \), \( s' \) and \( \omega \) are free parameters, and any choice of these parameters gives an eigenvector of \( U \), but \( s \) and \( s' \) are not independent once the vectors are normalized. The normalization \( \langle \psi_\lambda | \psi_\lambda \rangle = 1 \) imposes the constraints

\[
s' = \sqrt{\frac{|g_{01}(k')|^2 - (|g_{00}(k)|^2 + |g_{01}(k)|^2)s^2}{|g_{00}(k')|^2 + |g_{01}(k')|^2}} 
\]

\[
0 < s < s_{\text{max}} \quad \text{s}_{\text{max}} = \frac{|g_{01}(k')|}{\sqrt{|g_{00}(\lambda, k)|^2 + |g_{01}(k)|^2}} 
\]  

where the limit \( s \to s_{\text{max}} \) corresponds to \( s' \to 0 \). Any vector satisfying these relations is a normalized eigenvector of \( U \), but two eigenvectors with parameters \( \{s_1, s'_1, \omega_1\} \) and \( \{s_2, s'_2, \omega_2\} \) are not necessarily orthogonal to each other. But it is always possible to pick two orthogonal eigenvectors for each doubly degenerate eigenvalue, if these parameters satisfy

\[
s_2 = \sqrt{\frac{|g_{01}(k)|^2}{|g_{00}(k)|^2 + |g_{01}(k)|^2} - s_1^2} 
\]

\[
\omega_2 = \omega_1 + \pi. 
\]  

Any choice of \( s_1 \) and \( \omega_1 \) gives then an orthonormal pair of eigenvectors. Note that the weights \( s_1 \) can be different for each eigenvalue, as long as they fall on the interval given in Eq. (21).

The Bloch sphere representation of the reduced coin eigenvectors can now be constructed from Eq. (19) with the result

\[
r_x = -2 \text{Re}(\Theta) 
\]

\[
r_y = 2 \text{Im}(\Theta) 
\]

\[
r_z = s^2 \left(1 - \left|\frac{g_{00}(\lambda, k)}{g_{01}(k)}\right|^2\right) + s'^2 \left(1 - \left|\frac{g_{00}(\lambda, k')}{g_{01}(k')}\right|^2\right) 
\]  

where the function \( \Theta \) is defined as

\[
\Theta = s \frac{g_{00}(\lambda, k)}{g_{01}(k)} + s'^2 \frac{g_{00}(\lambda, k')}{g_{01}(k')} 
\]
Figure 2: Distribution of the reduced coin eigenvectors on the Bloch sphere for different values of the coin parameter $R$. The labeling of the markers is the same in all graphs. In graph c), the filled points correspond to $z=1$ and the unfilled points correspond to $z=2$. The weights between the conjugate components are set equal, $s'_i = s_i$, so that there is no difference between the $z$ components in a) and b). The system size is $N=20$ and $\alpha=0, \beta=0$.

The Bloch ball representation of the eigenvectors is plotted for different values of the coin parameters in Fig. 2, where we have moved to the spherical coordinates $(r_x, r_y, r_z) \rightarrow (r, \theta, \phi)$. The eigenvectors are distributed along well-defined trajectories, which become thicker as the number of lattice points increases, in analogy to the eigenvalue bands discussed in the previous section.

It can be seen from Fig. 2b) that for small values of $R$, the coin eigenstates are close to the equator where $\theta = \pi/2$, and increasing $R$ brings them closer to the poles of the Bloch ball. Fig. 2c) shows that the eigenstates with the same $k$ but different $z$ are at approximately same distance from the point $\phi = \pi$. The $z$ components of the eigenvectors traverse around the axis in opposite directions, with the angle $\phi$ increasing or decreasing depending on $z$. This is in contrast to the non-degenerate case, where the angle $\phi$ can be shown to be given by $\phi = \beta - \frac{\pi}{2} + 2\pi \frac{k}{N}$, i.e. independent of $z$. Note that the eigenvalues corresponding to $k = N/2 \pm \delta k$ are equal (see Fig. 1), and the eigenvectors for the same value are distributed at equal distance from the equator. These considerations hold when the weights $s$ and $s'$ are set equal in Eq. (19), and it should be noted that changing the parameter $s$ can also deform the trajectories, but these deformations are not explored here.

The degeneracy of the spectrum of $U$ is a signal of some kind of redundancy in its representation. This redundancy implies that there exists a non-trivial symmetry operator $S$ that leaves $U$ unchanged:

$$SU S^\dagger = U.$$  \hfill (28)
With the solutions for the eigenvectors of $U$, such a symmetry operator can be constructed by considering the orthogonal eigenvectors for each degenerate eigenvalue $\lambda(k,k',z)$. Since the operator $U$ is “blind” to the transitions between degenerate eigenstates $|\psi^1\rangle$ and $|\psi^2\rangle$, a non-trivial unitary operator that satisfies Eq. (28) is given by

$$S = \sum_{\lambda \in \Lambda_n} |\psi_\lambda\rangle\langle \psi_\lambda| + \sum_{\lambda \in \Lambda_d} \left( |\psi^2_\lambda\rangle\langle \psi^1_\lambda| + |\psi^1_\lambda\rangle\langle \psi^2_\lambda| \right)$$  \hspace{1cm} (29)$$

where $\Lambda_n$ is the set of non-degenerate eigenvalues (if any) and $\Lambda_d$ is the set of all degenerate eigenvalues. When written out explicitly, the operator $S$ consists of transitions between the left-moving and right-moving components $k$ and $k'$, and simultaneous rotations of the coin. It must therefore be understood as a joint symmetry which acts simultaneously on the position and coin degrees of freedom.

5 Protected eigenstates

Even if the rest of the spectrum is degenerate, in some cases the highest or the lowest eigenvalue might be unique, as seen for $k = 0$ and $k = N/2$ in Fig. (1a). Based on the discussion in the previous section, the eigenstates for unique and degenerate eigenvalues are characteristically different, since the latter are superpositions of two wavenumbers $k$ and $k'$. As seen in Fig. (2) the eigenvectors for the unique eigenvalues correspond to nodes of the trajectories in the Bloch ball, and these eigenvectors remain fixed as the value of $R$ changes.

The robustness of the special eigenvectors can be understood using the results from the previous section. According to Eqs. (14–15), the wavenumbers for degenerate eigenvalues are arranged into pairs $(m,n-m)$ where $m = \{0,1,\ldots,M\}$, and $(n+l,N-l)$ where $l = \{1,2,\ldots,L\}$. If $n$ is odd, $M = (n-1)/2$ and every wavenumber in the first group has a matching pair. But if $n$ is even, $M = n/2 - 1$ and the wavenumber $k = n/2$ does not have a pair, and the corresponding eigenvalue is unique. Similarly if $N - n$ is even, $L = (N-n)/2 - 1$ and the eigenvalue corresponding to $k = (N-n)/2$ (modulo $N$) is unique. The values of $k$ with a unique eigenvalue are summarized in the following table:

|   | $N$ even | $N$ odd |
|---|---------|---------|
| $n$ even | $k = \{n/2,(N-n)/2\}$ | $k = n/2$ |
| $n$ odd | $-\pi/2$ | $k = (N-n)/2$ |

For example in Fig. (1b), $n = 0$ and $N = 20$, and the eigenvalues at $k = 0$ and $k = 10$ are unique.

The widely used Hadamard coin is a curious special case in the parameter space. In the parameterization introduced in Eq. (1), it corresponds to the values $\{R,\alpha,\beta\} = \{1/2,3\pi/2,\pi/2\}$. If $N$ is an integer multiple of 4, this choice implies that the spectrum is degenerate and there are 2 unique eigenvalues in the spectrum, since the value $n = 3N/2$ is an even integer, see Eq. (15). If $N$ is an odd integer multiple of 2, the spectrum is fully degenerate since $n$ is an odd number. For odd $N$, the parameter $\alpha$ is not an integer multiple of $\pi/N$, and the spectrum is always non-degenerate.

The robustness of the eigenstates is explained by the behaviour of the matrix elements of $G$. Recall from last section that the components of the eigenstates for unique eigenvalues must satisfy Eq. (16). If $\alpha = n\pi/N$ and $k = n/2$, then $\alpha - 2\pi k/N = 0$ and it is easy to show that $g_{00}/g_{01} = (-1)^n e^{i(\alpha + \beta + 3\pi/2)}$. If $k = (N-n)/2$, then $\alpha - 2\pi k/N = \pi$ and it follows that $g_{00}/g_{01} = (-1)^n e^{i(-\alpha + \beta + \pi/2)}$. The eigenstates are thus equal superpositions of the coin components $|0\rangle$ and $|1\rangle$, with the phase difference determined only by the coin parameters $\alpha$ and $\beta$ (and the eigenvalue label $z$). This property is reflected in Fig. (2b) where the Bloch angle $\theta$ at $k = 0, N/2$ is equal to $\pi/2$ for all values of $R$. 


The robustness of the special eigenstates might be used to store quantum states and to protect them against arbitrary variations of the parameter $R$. If the eigenvalues $z = 1, 2$ at wavenumber $k$ are unique and the rest of the spectrum is degenerate, the eigenstates $|\Psi_{\lambda(k,1)}\rangle$ and $|\Psi_{\lambda(k,2)}\rangle$ remain “frozen” even if the parameter $R$ changes at every time step, as long as $R$ is spatially homogeneous and the parameters $\alpha$ and $\beta$ remain fixed. Therefore, if the initial state is

$$|\Psi(0)\rangle = x_0|\varphi\rangle + x_1|\Psi_{\lambda(k,1)}\rangle + x_2|\Psi_{\lambda(k,2)}\rangle$$  \hfill (30)$$

where $|\varphi\rangle$ is orthogonal to $|\Psi_{\lambda(k,1)}\rangle$ and $|\Psi_{\lambda(k,2)}\rangle$, the overlaps between the state at time $t$ and the eigenstates remain fixed at all times, up to a complex phase:

$$\langle \Psi_{\lambda(k,1)} | \Psi(t) \rangle = e^{iy_1}x_1$$  \hfill (31)$$

$$\langle \Psi_{\lambda(k,2)} | \Psi(t) \rangle = e^{iy_2}x_2,$$$\hfill (32)$$

and the probabilities to measure the states $|\Psi_{\lambda(k,1)}\rangle$ and $|\Psi_{\lambda(k,2)}\rangle$ are constant. The quantum walk can thus act as a memory which is protected from temporal variations of $R$.

The robustness of the protected states is reminiscent of symmetry-protected topological phases, where the edges between different phases may host chiral states inside the band gap. Such states are also robust to arbitrary variations of the system parameters, as long as the symmetry class of the Hamiltonian does not change. Such states have also been found in the so-called split-step quantum walk [27, 28] and also in disordered quantum walks [29]. In fact, the topological structure of quantum walks has been found to be richer than that of non-interacting many-body systems, and the topological features in the quantum walk are not always captured by standard tools used to characterize topological phases in non-interacting systems [30]. In the simple case that we have considered here, the properties of the eigenstates were found to be very different in the presence of symmetry. The topological features in quantum walks are still not completely understood, and it interesting that even the simplest quantum walk can host states which are robust against certain variations of the system parameters.

6 Conclusions

The spectrum of the time evolution operator of discrete-time quantum walks was analysed for a general 2-dimensional unitary coin. The eigenvalues are labelled by two integers $k$ and $z$, where $k$ is the wavenumber in Fourier space and $z$ labels the upper and lower quasi-energy bands. If the coin is parameterized suitably, each parameter can be associated with distinct properties of the spectrum. The bias parameter $R$ controls the dispersion of the bands, the angle $\alpha$ changes the symmetry between left-moving and right-moving components, and the angle $\beta$ sets just the base level of the quasi-energies.

For the eigenstates, the geometric picture using the Bloch ball was found to be very useful. The reduced eigenvectors in coin space are distributed along well-defined trajectories, which become deformed as the coin parameters are varied. For small values of the bias parameter $R$, the eigenvectors remain close to the equator. Increasing $R$ brings them closer to the poles, with all eigenvectors localized at either $c = 0$ or $c = 1$ when $R = 1$. If the parameter $\alpha$ is an integer multiple $\pi/N$, the spectrum becomes degenerate, which has a significant impact on the eigenstates. In the non-degenerate case, the eigenvectors are product states of the Fourier modes and coin states, but in the presence of degeneracy they are entangled superpositions of conjugate wavenumbers $k$ and $k'$. In the latter case the reduced coin states are mixed states, and they are not constrained to the surface of the Bloch sphere. The representation of the eigenvectors is also not unique in this case, and we have identified the parameters $s_1$ and $\omega_1$ as a certain kind gauge freedom,
which can be chosen freely while the resulting states are still orthonormal eigenstates of $U$. However, the Bloch representation of the eigenvectors is not equal for different $s_1$ and $\omega_1$.

Finally, depending on the evenness of the number of lattices sites $N$ and the difference $(N - n)$, where $\alpha = n\pi/N$, it has been shown that there may exist unique eigenvalues in the degenerate spectrum. These points are located at the top or bottom of the quasi-energy bands, and the eigenstates corresponding to the unique eigenvalues are robust against arbitrary variations in the parameter $R$. If the initial state of the quantum walk has a non-zero overlap with such states, the overlap will remain constant in time, even if the parameter $R$ changes between time steps. Since these states remain constant in time, they might be useful for storing quantum states, and such a memory would be protected from arbitrary temporal variations in the parameter $R$.

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