Edge States of a Periodic Chain with Four-Band Energy Spectrum

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Tight-binding model on a finite chain is studied with four-fold alternated hopping parameters \( t_{1,2,3,4} \). Imposing the open boundary conditions, the corresponding recursion is solved analytically with special attention paid to the occurrence of edge states. Corresponding results are strongly corroborated by numeric calculations. It is shown that in the system there exist four different edge phases if the number of sites is odd, and eight edges phases if the chain comprises even number of sites. Phases are labelled by \( \sigma_1 \equiv \text{sgn}(t_1 t_3 - t_2 t_4) \), \( \sigma_2 \equiv \text{sgn}(t_1 t_4 - t_2 t_3) \) and \( \sigma_3 \equiv \text{sgn}(t_1 t_2 - t_3 t_4) \). It is shown that these quantities represent gauge invariant topological indices emerging in the corresponding infinite chains.

1. Introduction

The most significant imprint of the topological order exhibited by topological insulators \cite{1-3} is the occurrence of edge states. The simplest construction producing topological phases is the Su-Schrieffer-Heeger (SSH) model originally introduced for describing the polyacetylene \cite{4}, and later on revisited in connection with topological insulators. The SSH model exploits 1D tight-binding Hamiltonian with doubly alternated hopping parameters \( t_{1,2} \) between the nearest neighboring sites and produces two energy bands separated by a gap \( |t_1 - t_2| \). Correspondingly, the two topologically distinct phases occur, and the transition between those two takes place at \( t_1 = t_2 \) accompanied by closing and reopening the gap.

In the present paper we generalize the SSH model with the aim of detecting more diverse topological content than the two-phase one. Similar attempt by involving the next-to-nearest hoppings has been carried out in Ref. \cite{5} leading to the phase diagram identical to the one of Haldane model \cite{6}. We study alternative modification keeping the nearest neighbour hoppings only, but with four-fold alternated amplitudes \( t_{1,2,3,4} \). The corresponding energy spectrum consists of four bands separated by independently controlled gaps. Since the closing and reopening of a gap is associated with topological phase transitions, one may expect the occurrence of more rich topological content. In this scope we study a chain comprising finite number \( N \) of sites, and find 4 and 8 different phases for \( N = \text{odd} \) and \( N = \text{even} \), respectively.

The 8 phases (for \( N = \text{even} \)) are labelled by \( (\sigma_1, \sigma_2, \sigma_3) \) where

\[
\begin{align*}
\sigma_1 &\equiv \text{sgn}(t_1 t_3 - t_2 t_4), \\
\sigma_2 &\equiv \text{sgn}(t_1 t_4 - t_2 t_3), \\
\sigma_3 &\equiv \text{sgn}(t_1 t_2 - t_3 t_4),
\end{align*}
\]

which are gauge invariant topological indices emerging in the corresponding infinite chains. The 4 phases emerging in the case of \( N = \text{odd} \) are labelled by \( (\sigma_1, \sigma_2) \).

In Sec. 2 we present finite SSH model for demonstrating the technique \cite{8} of solving periodic three-term recurrence relation analytically in terms of Chebyshev polynomials. In Sec. 3 the technique is applied to the four-band model. Analytic results are corroborated by numeric calculations. In Sec. 4 we introduce certain scheme for constructing Berry curvature for 1D periodic infinite chains. In the case of SSH (two-band) model the scheme gives out the Zak phase \cite{8}, while in four-band model reconstructs the aforementioned labels \( \sigma_{1,2,3} \) as gauge invariant topological indices. Results are summarized in Sec. 5. Calculational details are placed in Appendix.

Chebyshev \( U \)-polynomials can be applied to 2D periodic lattices as well \cite{9}. Alternative analytic approach to the issue of edge modes can be found in Ref. \cite{10}.

2. Two-Band Finite Chain

Finite chain with doubly alternated hoppings between the nearest sites is set by the tight-binding Hamiltonian

\[
H = - \sum_{n=1}^{N-1} t_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})
\]

where \( N \) is the number of sites. Hopping parameters are periodic \( t_{n+2} = t_n \) and can be put all positive.

The corresponding one-particle problem reads

\[
\begin{pmatrix}
t c_{t_1} & 0 & 0 & \cdots & 0 \\
t c_{t_2} & 0 & 0 & \cdots & 0 \\
0 & t c_{t_1} & 0 & \cdots & 0 \\
0 & 0 & t c_{t_2} & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & t
\end{pmatrix}
\begin{pmatrix}
\psi_{1} \\
\psi_{2} \\
\psi_{3} \\
\psi_{4} \\
\vdots \\
\psi_{N}
\end{pmatrix} = 0.
\]

In the component form this system appears as

\[
t_n \psi_n + c \psi_{n+1} + t_{n+1} \psi_{n+2} = 0
\]

supplied by the boundary conditions \( \psi_0 = \psi_{N+1} = 0 \).

Solution to (3) appears as (see Appendix A for details)

\[
\psi_{2n+1} = [U_n(\xi) + (t_2/t_1)U_{n-1}(\xi)]\psi_1
\]

\[
\psi_{2n+2} = -(c/t_1)U_n(\xi)\psi_1
\]

where

\[
\xi(t_1, t_2) = \left((c^2 - t_1^2 - t_2^2)/2t_1 t_2\right)
\]

and \( U_n \) are the Chebyshev polynomials of the second kind.
In (4) all \( \psi_n \) are expressed via \( \psi_1 \). This is appropriate for describing the edge states localized at left edge \((n = 1)\). For the states localized at the right edge \((n = N)\) it is more convenient to express \( \psi_n \) via \( \psi_N \). For this purpose we introduce \( \psi_n = \phi_{N-n+1} \) and \( t_n = u_{N-n} \). Then the recurrence (3) takes the form

\[
u_n \phi_n + c \phi_{n+1} + u_n \phi_{n+2} = 0 \tag{6}
\]

accompanied by \( \phi_0 = \psi_{N+1} = 0 \), and the solutions to (6) can be obtained by performing replacements \( t_n \rightarrow u_n \) and \( \psi_n \rightarrow \phi_n \) in (4) and (5). We have \( u_{1,2} = t_{1,2} \) for \( N = \text{even} \), and \( u_{1,2} = t_{2,1} \) for \( N = \text{odd} \). Irrespectively of these options one finds \( u_1^2 + u_2^2 = t_1^2 + t_2^2 \) and \( u_1 u_2 = t_1 t_2 \), where from we have \( \xi(u_1, u_2) = \xi(t_1, t_2) \), and the solution to (6) appears as

\[
\begin{align*}
\phi_{2n+1} &= \left[ U_n(\xi) + (u_2/u_1)U_{n-1}(\xi) \right] \psi_N, \\
\phi_{2n+2} &= -(c/u_1)U_n(\xi) \phi_1.
\end{align*}
\tag{7a}
\]

Rewriting these in terms of \( \phi_n = \psi_{N-n+1} \) we come to

\[
\begin{align*}
\psi_{N-2n} &= \left[ U_n(\xi) + (u_2/u_1)U_{n-1}(\xi) \right] \psi_N, \\
\psi_{N-2n-1} &= -(c/u_1)U_n(\xi) \psi_N,
\end{align*}
\tag{8a}
\]

where the concrete connection between \( u_n \) and \( t_n \) depends on the number of sites, but \( \xi \) is the same as given by (5).

Bulk-edge properties of eigenstates can be specified by the value of \( \xi \). For \( |\xi| < 1 \) we put \( \xi = \cos \gamma \) and using

\[
U_n(\cos \gamma) = \frac{\sin((n + 1)/2 \gamma)}{\sin \gamma} \tag{9}
\]

find that \( \psi_n \) oscillates with respect to \( n \), hence it is a bulk state.

For \( |\xi| > 1 \) we put \( \xi = \cosh \gamma \) and use

\[
U_n(\pm \cos \gamma) = (\pm 1)^n \frac{\sinh((n + 1)/2 \gamma)}{\sinh \gamma}. \tag{10}
\]

Here we may have edge states due to the factors of \( e^{\pm nx} \).

Taking \( n = -1 \) in (4b), the boundary condition \( \psi_0 = 0 \) is automatically satisfied due to \( U_{-1}(x) = 0 \), while the other one \( \psi_{N+1} = 0 \) takes the role of secular equation and determines the energy spectrum. Depending on the value of \( N \), it appears as \( (N) \) is an integer

\[
\begin{align*}
N = 2J + 1: & \quad c U_{J}(\xi) = 0, \\
N = 2J + 2: & \quad U_{J+1}(\xi) + (t_2/t_1)U_{J}(\xi) = 0.
\end{align*}
\tag{11a}
\]

Similarly, taking \( n = -1 \) in (8b) we find that \( \psi_{N+1} = 0 \) is automatically satisfied and the other boundary condition takes the role of secular equation leading to the same (11).

2.1. Edge States for \( N = 2J + 1 \)

Secular equation (11a) breaks into two equations \( c = 0 \) and \( U_{J}(\xi) = 0 \). Solutions to the later gives \( |\xi| < 1 \) since the roots of \( U_n(x) \) are all located in the interval \((0, 1)\). Hence the states determined by \( U_{J}(\xi) = 0 \) are bulk states and we turn to \( c = 0 \).

Taking \( c = 0 \) in (5) we find \( \xi = -\frac{1}{2}(t_1/t_2) - \frac{1}{2}(t_2/t_1) < -1 \), i.e. these are edge states in accord with (10).

For \( t_1 < t_2 \) we put \( \xi = -\cosh \gamma \) and resolve as \( e^{-\gamma} = t_1/t_2 \). Using this in (4) we come to

\[
\begin{align*}
\psi_{2n+1} &= (-t_1/t_2)^n \psi_1, \\
\psi_{2n+2} &= 0,
\end{align*}
\tag{12a}
\]

which is localized at the left edge.

For \( t_1 > t_2 \) we put \( \xi = -\cosh \gamma \) and resolve as \( e^{-\gamma} = t_2/t_1 \). Using in (8) we come to

\[
\begin{align*}
\psi_{2n+1} &= (-t_2/t_1)^{J-n} \psi_N, \\
\psi_{2n+2} &= 0,
\end{align*}
\tag{13a}
\]

which is localized at the right edge.

Occurrence of a zero mode for \( N = \text{odd} \) is a general fact: amount of zero modes in bipartite chains is \([N_1 - N_2] \) with \( N_{1,2} \) the numbers of sites in two sublattices \([11]\).

2.2. Edge States for \( N = 2J + 2 \)

We search for the edge states provided \( J \rightarrow \infty \). For this purposes we study the equation (11b). As already pointed out, the edge states emerge only in the cases when \( |\xi| > 1 \).

\( \xi > 1 \). In this case we put \( \xi = \cosh \gamma \) and rewrite (11b) as

\[
\frac{\sinh((J+1)/2 \gamma)}{\sinh(J/2 \gamma)} \cdot \frac{t_2}{t_1} = 0.
\tag{14}
\]

Assuming \( z > 0 \), and taking the limit \( J \rightarrow \infty \) we obtain

\[
e^{-2z} + (t_1/t_2) = 0
\]

with no solution since \( t_{1,2} > 0 \) (pointed out earlier), hence \( \xi > 1 \) cannot be realized.

\( \xi < -1 \). We then put \( \xi = -\cosh \gamma \) and rewrite (11b) as

\[
\frac{\sinh((J+1)/2 \gamma)}{\sinh(J/2 \gamma)} \cdot \frac{t_2}{t_1} = 0.
\tag{16}
\]

Assuming \( z > 0 \), and taking the limit \( J \rightarrow \infty \) we obtain

\[
e^{-2z} = t_1/t_2
\tag{17}
\]

which (due to \( z > 0 \)) may be realized only for \( t_1 < t_2 \).

Combining (17) with (5) we come to \( c^2 = 0 \). The fact that the zero-mode occurs as \( c^2 = 0 \) signifies the energy level is doubly degenerated. One wave function is obtained by use of (4) and appears as

\[
\begin{align*}
\psi_{2n+1} &= (-t_1/t_2)^n \psi_1, \\
\psi_{2n+2} &= 0,
\end{align*}
\tag{18a}
\]

representing the left edge state (localized at \( \psi_1 \)).

The other is obtained by use of (8) and gives

\[
\begin{align*}
\psi_{2n+2} &= (t_1/t_2)^{J-n} \psi_N, \\
\psi_{2n+1} &= 0,
\end{align*}
\tag{19a}
\]

representing the right edge state (localized at \( \psi_N \)).
2.3. Numeric Calculations

In support of the above analytic expressions below we bring the results of numeric calculations for \( N = 101 \) and \( N = 102 \). The overall magnitude of \( t_{1,2} \) is irrelevant and we parameterize as \( t_1 = \sin \theta \) and \( t_2 = \cos \theta \). The energy spectra versus \( \theta \) set by (2) are shown in Fig. 1.

![Energy spectra](image)

**FIG. 1:** Energy spectra \( |c_1, \ldots, c_{101}| \) (left) and \( |c_1, \ldots, c_{102}| \) (right) vs \( \theta \) obtained by numeric calculations for \( N = 101 \) and \( N = 102 \), respectively. For \( N = \text{odd} \) the single zero mode develops for any \( t_1 \) and \( t_2 \). For \( N = \text{even} \) doubly degenerated zero mode develops only for \( t_1 < t_2 \).

3. Four-Band Finite Chain

We pass to a finite chain with four-fold alternated hoppings. The corresponding one-particle equation reads as

\[
\begin{bmatrix}
\epsilon & t_1 & 0 & 0 & 0 & \cdots & 0 & \psi_1 \\
t_1 & \epsilon & t_2 & 0 & 0 & \cdots & 0 & \psi_2 \\
0 & t_2 & \epsilon & t_3 & 0 & \cdots & 0 & \psi_3 \\
0 & 0 & t_3 & \epsilon & t_4 & \cdots & 0 & \psi_4 \\
0 & 0 & 0 & t_4 & \epsilon & t_1 & \cdots & \psi_5 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \cdots & \cdots & \psi_6 \\
0 & 0 & 0 & 0 & 0 & \cdots & \epsilon \\
\end{bmatrix}
= 0. \quad (20)
\]

In the component form this system appears as

\[
t_n \psi_n + \epsilon \psi_{n+1} + t_{n+1} \psi_{n+2} = 0 \quad \text{(21)}
\]

with \( t_{n+4} = t_n \), and are supplied by \( \psi_0 = \psi_{N+1} = 0 \). In accord with Ref. [7] we write the solution to (21)

\[
\psi_{4n+1} = \left[ U_n(\xi) + \frac{t_4}{t_3} \frac{\epsilon^2 - t_2^2}{t_1} U_{n-1}(\xi) \right] \psi_1, \quad (22a)
\]

\[
\psi_{4n+2} = -\epsilon \left[ U_n(\xi) + \frac{t_1 t_4}{t_2 t_3} U_{n-1}(\xi) \right] \psi_1, \quad (22b)
\]

\[
\psi_{4n+3} = \left[ \frac{\epsilon^2 - t_2^2}{t_1 t_2} U_n(\xi) + \frac{t_4}{t_3} U_{n-1}(\xi) \right] \psi_1, \quad (22c)
\]

\[
\psi_{4n+4} = -\epsilon \left[ \frac{\epsilon^2 - t_2^2}{t_1 t_2 t_3} U_n(\xi) \right] \psi_1, \quad (22d)
\]

where

\[
\xi = \frac{\epsilon^4 - (t_1^2 + t_2^2 + t_3^2 + t_4^2) \epsilon^2 + t_1^2 t_2^2 + t_2^2 t_3^2 + t_3^2 t_4^2}{2 t_1 t_2 t_3 t_4}. \quad (23)
\]

Alternatively, we can express \( \psi_n \) in terms of \( \psi_N \). Introducing \( \psi_n = \phi_{N-n+1} \) and \( t_n = u_{N-n} \) we rewrite (21) as

\[
u_n \psi_n + c \psi_{n+1} + u_{n+1} \psi_{n+2} = 0 \quad \text{(24)}
\]

accompanied by \( \phi_0 = \phi_{N+1} = 0 \).

Solution to (24) can be written by replacing \( t_n \rightarrow u_n \) and \( \psi_n \rightarrow \phi_n \) in (22) and (23). The parameter \( \xi \) defined by (23) is invariant with respect to \( t_n \rightarrow u_n \), and we come to

\[
\psi_{N-4n} = \left[ \frac{u_4 \epsilon^2 - u_2^2}{u_3} U_{n-1}(\xi) \right] \psi_N, \quad (25a)
\]

\[
\psi_{N-4n-1} = -\epsilon \left[ U_n(\xi) + \frac{u_1 u_4}{u_2 u_3} U_{n-1}(\xi) \right] \psi_N, \quad (25b)
\]

\[
\psi_{N-4n-2} = \epsilon^2 - u_2^2 U_n(\xi) + \frac{u_4}{u_3} U_{n-1}(\xi) \psi_N, \quad (25c)
\]

\[
\psi_{N-4n-3} = -\epsilon \left[ \frac{\epsilon^2 - u_2^2}{u_1 u_2 u_3} U_n(\xi) \right] \psi_N, \quad (25d)
\]

where the connection between \( u_n \) and \( t_n \) depends on \( N \).

Taking \( n = -1 \) in (22d) the condition \( \psi_0 = 0 \) is automatically satisfied due to \( U(-x) = 0 \), while the one \( \psi_{N+1} = 0 \) appears as

\[
N = 4J + 1: \quad \epsilon \left[ t_2 t_3 U_1(\xi) + t_1 t_4 U_{J-1}(\xi) \right] = 0, \quad (26a)
\]

\[
N = 4J + 2: \quad t_1(\epsilon^2 - t_2^2) U_J(\xi) + t_2 t_3 t_4 U_{J-1}(\xi) = 0, \quad (26b)
\]

\[
N = 4J + 3: \quad \epsilon(\epsilon^2 - t_2^2) U_J(\xi) = 0, \quad (26c)
\]

\[
N = 4J + 4: \quad t_1 t_2 t_3 U_{J+1}(\xi) + t_4(\epsilon^2 - t_2^2) U_J(\xi) = 0, \quad (26d)
\]

and determines the energy eigenvalues.

Taking \( n = -1 \) in (25d) we find \( \psi_{N+1} = 0 \) is automatically satisfied, \( \psi_0 = 0 \) leads to the same (26).

In the following four subsections we separately present the cases \( N = 4J + j \) with \( j = 1, 2, 3, 4 \). In order expressions to be compact, hereafter we put \( \psi_1 = 1 \) and \( \psi_N = 1 \) for the left and right edge states respectively, and indicate only non-vanishing components of \( \psi_n \).

3.1. Edge States for \( N = 4J + 1 \)

Calculated details are collected in Appendix B, while here we show the results.

For \( t_1 t_3 < t_2 t_4 \) one left edge state occurs

\[
\epsilon = 0, \quad \left\{ \begin{array}{l}
\psi_{4n+1} = (t_2 t_4 t_1 t_3)^n \\
\psi_{4n+3} = -(t_1 t_2) (t_1 t_3 t_2 t_4)^n.
\end{array} \right. \quad (27)
\]

For \( t_1 t_3 > t_2 t_4 \) we have one right edge state

\[
\epsilon = 0, \quad \left\{ \begin{array}{l}
\psi_{4n+1} = (t_2 t_3 t_1 t_4)^{n-1} \\
\psi_{4n+3} = -(t_1 t_2 t_3 t_4)^{n-1}.
\end{array} \right. \quad (28)
\]

For \( t_1 t_4 > t_2 t_3 \) we have four edge states. Two states out of those four are localized at \( n = 1 \) and appear as

\[
\epsilon = \pm (t_1^2 + t_2^2)^{1/2}, \quad \left\{ \begin{array}{l}
\psi_{4n+1} = (t_2 t_3 t_1 t_4)^n, \\
\psi_{4n+2} = -(t_1 t_3 t_2 t_4)^n, \\
\psi_{4n+3} = (t_2 t_1)(t_3 t_4)^n, \\
\psi_{4n+4} = (t_1 t_2 t_3 t_4)^n.
\end{array} \right. \quad (29a)
\]
The other two are localized at \( n = N \) and look as

\[
\epsilon = \pm (t_3^2 + t_4^2)^{1/2}, \quad \begin{cases} 
\psi_{4n+1} = (-t_2t_3/t_1t_4)^{d-n}, \\
\psi_{4n+3} = (t_3/t_4)(-t_2t_3/t_1t_4)^{d-n-1}, \\
\psi_{4n} = -(e/t_4)(-t_2t_3/t_1t_4)^{d-n}.
\end{cases}
\] (29b)

Introduce \( \sigma_1 \equiv \text{sgn}(t_1t_3 - t_2t_4) \) and \( \sigma_2 \equiv \text{sgn}(t_1t_4 - t_2t_3) \). We then label the 4 phases by \((\sigma_1, \sigma_2)\) as follows

\[
\begin{align*}
A \ (-,-) &: \text{ 1 edge state (27)}, \\
B \ (-,+): & \text{ 5 edge states (27), (29)}, \\
C \ (+,-) &: \text{ 1 edge state (28)}, \\
D \ (+,+): & \text{ 5 edge states (28), (29)}.
\end{align*}
\]

In order to confirm the analytic expressions, we present the numerically obtained energy spectra for \( N = 101 \). We parameterize \( t_{1,2,3,4} \) as (overall magnitude irrelevant)

\[
\begin{align*}
t_1 &= \cos \theta_3 \sin \theta_1, & (30a) \\
t_2 &= \cos \theta_3 \cos \theta_1, & (30b) \\
t_3 &= \sin \theta_3 \cos \theta_2, & (30c) \\
t_4 &= \sin \theta_3 \sin \theta_2. & (30d)
\end{align*}
\]

In Fig. 2 we present the energy spectrum \( \epsilon_{1-101} \) versus \( \theta_1 \) with \( \theta_2 = \frac{\pi}{8} \) and \( \theta_3 = \frac{\pi}{16} \). For \( \theta_1 < \theta_2 \) the system is found in phase A. Increasing \( \theta_1 \) we observe the transition into phase C at \( \theta_1 = \theta_2 \), and subsequently into phase D at \( \theta_1 = \frac{\pi}{2} - \theta_2 \). Thus the width of phase C laying in between the phases A and D is \( \frac{\pi}{2} - 2\theta_2 \).

![FIG. 2: Energy spectrum \( \epsilon_{1-101} \) vs \( \theta_1 \) for \( \theta_2 = \frac{\pi}{8} \) and \( \theta_3 = \frac{\pi}{16} \).](image)

We comment on how the dispersion shown in Fig. 2 is affected by varying \( \theta_2 \). Increasing \( \theta_2 \) the phase C shrinks and disappears at \( \theta_2 = \frac{\pi}{4} \). In that case the system passes from phase A right into D. Further increase of \( \theta_2 \) cause the phases A and D become separated again, but with phase B in between as shown in Fig. 3.

![FIG. 3: Energy spectrum \( \epsilon_{1-101} \) vs \( \theta_1 \) for \( \theta_2 = \frac{3\pi}{8} \) and \( \theta_3 = \frac{\pi}{16} \).](image)

We discuss the role of \( \theta_3 \). In Fig. 2 and Fig. 3 there are gaps due to \((t_3^2 + t_4^2)^{1/2} > (t_1^2 + t_2^2)^{1/2}\). The later results from \( \theta_3 < \frac{\pi}{4} \) (see (30)). The gaps close at \( \theta_3 = \frac{\pi}{4} \), as depicted in Fig. 4 with \( \theta_2 = \frac{\pi}{8} \) (top) and \( \frac{3\pi}{8} \) (bottom). Behaviour with respect to \( \theta_2 \) is the same, as already stated.

![FIG. 4: \( \epsilon_{1-101} \) vs \( \theta_1 \) for \( \theta_3 = \frac{1\pi}{4} \), \( \theta_2 = \frac{1\pi}{8} \) (top), \( \theta_2 = \frac{3\pi}{8} \) (bottom).](image)
Further increase of $\vartheta_3$ result in reopening the gaps with the only difference that we have $(t_3^2 + t_4^2)^{1/2} > (t_2^2 + t_4^2)^{1/2}$ due to $\vartheta_3 > \frac{3}{4} \pi$ (see (30)).

3.2. Edge States for $N = 4J + 2$

For $t_1 t_3 < t_2 t_4$ we have two edge states (Appendix C)

$\epsilon = 0, \begin{cases} \varphi_{4n+1} = (t_1 t_3/t_2 t_4)^n \varphi, \\ \varphi_{4n+3} = -(t_1 t_2)(t_1 t_3/t_2 t_4)^n \varphi \end{cases}$ \hspace{0.5cm} (31a)

$\epsilon = 0, \begin{cases} \varphi_{4n+2} = (t_1 t_3/t_2 t_4)^{2n-3} \varphi, \\ \varphi_{4n+4} = -(t_1 t_2)(t_1 t_3/t_2 t_4)^{2n-3} \varphi \end{cases}$ \hspace{0.5cm} (31b)

localized at left and right edges, respectively.

For $t_1 t_3 > t_2 t_4$ we have two edge states

$\epsilon = \pm (t_1^2 + t_2^2)^{1/2}, \begin{cases} \varphi_{4n+1} = (t_2 t_3/t_1 t_4)^n \varphi, \\ \varphi_{4n+2} = (t_2 t_3/t_1 t_4)^{2n-3} \varphi, \\ \varphi_{4n+3} = (t_2 t_4/(t_2 t_3/t_1 t_4))^{n-1} \varphi \end{cases}$ \hspace{0.5cm} (32)

For $t_1 t_2 > t_3 t_4$ we have two edge states

$\epsilon = \pm (t_1^2 + t_4^2)^{1/2}, \begin{cases} \varphi_{4n+1} = (t_3 t_4/t_1 t_2)^n \varphi, \\ \varphi_{4n+2} = (t_3 t_4/t_1 t_2)^{2n-3} \varphi, \\ \varphi_{4n+3} = (t_3 t_4/(t_3 t_4/t_1 t_2))^{n-1} \varphi \end{cases}$ \hspace{0.5cm} (33)

Here we employ three parameters $\sigma_1 \equiv \text{sgn}(t_1 t_3 - t_2 t_4)$, $\sigma_2 \equiv \text{sgn}(t_1 t_4 - t_3 t_2)$, $\sigma_3 \equiv \text{sgn}(t_1 t_2 - t_3 t_4)$ and label the eight (= $2^3$) phases by $(\sigma_1, \sigma_2, \sigma_3)$ as follows

1. $(-, -, -)$: 2 edge states (31),
2. $(-, +, +)$: 4 edge states (31), (33),
3. $(-, +, -)$: 4 edge states (31), (32),
4. $(+, +, +)$: 6 edge states (31), (32), (33),
5. $(+, +, -)$: no edge states,
6. $(+, +, +)$: 2 edge states (33),
7. $(+, +, +)$: 2 edge states (32),
8. $(+, +, +)$: 4 edge states (32), (33).

Fig. 5 depicts the spectrum versus $\vartheta_1$ with $\vartheta_2 = \frac{3}{8} \pi$ and $\vartheta_3 = \frac{3}{16} \pi$.

Increasing $\vartheta_2$, the width of phase $\varpi$ ($\frac{3}{4} \pi - 2\vartheta_2$) shrinks and disappears at $\vartheta_2 = \frac{3}{8} \pi$, so that the phase $\Xi$ becomes followed right by $\Sigma$. Further increase of $\vartheta_2$ causes the phases $\Xi$ and $\Omega$ become detached again, but with $\Xi$ instead of $\varpi$ in between as shown in Fig. 6.

Dependence on $\vartheta_3$ is analogous to the case of $N = 4J + 1$. Namely, for $\vartheta_3 < \frac{1}{8} \pi$ (Fig. 5 and Fig. 6) the two bunches of positive (negative) levels are separated by the gap, but with the levels $\pm (t_4^2 + t_2^2)^{1/2}$ in between. Increasing $\vartheta_3$ we find that for $\vartheta_3 = \frac{1}{8} \pi$ the gaps close and for $\vartheta_3 > \frac{1}{8} \pi$ the edge states are lost.

3.3. Edge States for $N = 4J + 3$

For $t_1 t_3 < t_2 t_4$ we have the left edge state (Appendix D)

$\epsilon = 0, \begin{cases} \varphi_{4n+1} = (t_1 t_3/t_2 t_4)^n \varphi, \\ \varphi_{4n+3} = -(t_1 t_2)(t_1 t_3/t_2 t_4)^n \varphi \end{cases}$ \hspace{0.5cm} (34)
For $t_1 t_3 > t_2 t_4$ we have the right edge state
\[ \epsilon = 0, \quad \begin{cases} \psi_{4n+1} = (t_2 t_4 / t_1 t_3)^{n-1}, \\ \psi_{4n+2} = (t_2 t_4 / t_1 t_3)^{n-1}. \end{cases} \] (35)

For $t_1 t_4 > t_2 t_3$ we have two left edge states
\[ \epsilon = \pm (t_1^2 + t_2^2)^{1/2}, \quad \begin{cases} \psi_{4n+1} = (t_2 t_3 / t_1 t_4)^n, \\ \psi_{4n+2} = (-t_2 t_3 / t_1 t_4)^n, \\ \psi_{4n+3} = (t_2 t_3 / t_1 t_4)^n, \\ \psi_{4n+4} = (-t_2 t_3 / t_1 t_4)^n. \end{cases} \] (36)

and for $t_1 t_4 < t_2 t_3$ we have two right edge states
\[ \epsilon = \pm (t_1^2 + t_2^2)^{1/2}, \quad \begin{cases} \psi_{4n+1} = (-t_1 t_4 / t_2 t_3)^{n-1}, \\ \psi_{4n+2} = (t_1 t_4 / t_2 t_3)^{n-1}, \\ \psi_{4n+3} = (t_1 t_4 / t_2 t_3)^{n-1}. \end{cases} \] (37)

Using $\sigma_1 = \text{sgn}(t_1 t_3 - t_2 t_4)$ and $\sigma_2 = \text{sgn}(t_1 t_4 - t_2 t_3)$ as in the case of $N = 4J + 1$, we label the 4 phases by $A, B, C, D$ with respect to $(\sigma_1, \sigma_2)$.

Properties of spectra with respect to $\theta_2$ and $\theta_3$ are the same as for $N = 4J + 1$. Therefore, in Fig. 8 we show only couple of cases ($\theta_2, \theta_3 = (\frac{3}{8} \pi, \frac{3}{10} \pi)$) and ($\theta_2, \theta_3 = (\frac{3}{8} \pi, \frac{7}{10} \pi)$).

![Figure 8](image)

FIG. 8: The spectrum $c_{1-103}$ vs $\theta_1$ for ($\theta_2, \theta_3 = (\frac{3}{8} \pi, \frac{3}{10} \pi)$) (top) and ($\theta_2, \theta_3 = (\frac{3}{8} \pi, \frac{7}{10} \pi)$) (bottom).

In the top panel we have $\theta_2 < \frac{1}{4} \pi$ and consequently the phase $C$ occurs in between $A$ and $D$. For $\theta_2 > \frac{1}{4} \pi$ the intermediate phase disappears and reappears as $B$ for $\theta_2 > \frac{1}{4} \pi$ in the bottom panel.

For $\theta_3 < \frac{1}{4} \pi$ (top) there are gaps, which close at $\theta_3 = \frac{1}{4} \pi$ and reopen for $\theta_3 > \frac{1}{4} \pi$ (bottom). After reopening the gaps the edge state levels $\epsilon = \pm (t_1^2 + t_2^2)^{1/2}$ initially attached to the outer bands (top panel) become attached to the inner ones (bottom panel).

### 3.4. Edge States for $N = 4J + 4$

For $t_1 t_3 < t_2 t_4$ we have two edge states (see Appendix E). One is the left edge state and appears as
\[ \epsilon = 0, \quad \begin{cases} \psi_{4n+1} = (t_1 t_3 / t_2 t_4)^n, \\ \psi_{4n+3} = - (t_1 t_3 / t_2 t_4)^n. \end{cases} \] (38a)

The other is the right edge state and looks as
\[ \epsilon = 0, \quad \begin{cases} \psi_{4n+1} = (t_1 t_3 / t_2 t_4)^{n-1}, \\ \psi_{4n+2} = -(t_3 / t_4)(t_1 t_3 / t_2 t_4)^{n-1}. \end{cases} \] (38b)

For $t_1 t_4 > t_2 t_3$ we have
\[ \epsilon = \pm (t_1^2 + t_2^2)^{1/2}, \quad \begin{cases} \psi_{4n+1} = (t_1 t_4 / t_2 t_3)^n, \\ \psi_{4n+2} = (t_1 t_4 / t_2 t_3)^n, \\ \psi_{4n+3} = (-t_1 t_4 / t_2 t_3)^n, \\ \psi_{4n+4} = (t_1 t_4 / t_2 t_3)^n. \end{cases} \] (39)

For $t_3 t_4 > t_1 t_2$ we have
\[ \epsilon = \pm (t_3^2 + t_4^2)^{1/2}, \quad \begin{cases} \psi_{4n+1} = (-t_2 t_4 / t_1 t_3)^n, \\ \psi_{4n+2} = (t_2 t_4 / t_1 t_3)^n, \\ \psi_{4n+3} = (-t_2 t_4 / t_1 t_3)^n, \\ \psi_{4n+4} = (t_2 t_4 / t_1 t_3)^n. \end{cases} \] (40)

Here we have the same defining parameters ($\sigma_1, \sigma_2, \sigma_3$) as in the case of $N = 4J + 2$, hence 8 phases, labelled by $\circ \oplus \oplus$ with respect to the values of ($\sigma_1, \sigma_2, \sigma_3$) as for $N = 4J + 2$.

![Figure 9](image)

FIG. 9: Energy spectrum $c_{1-104}$ vs $\theta_1$ for $\theta_2 = \frac{1}{8} \pi$ and $\theta_3 = \frac{3}{10} \pi$. 
Plotting the spectra here we use the parametrization

\[ t_1 = \cos \theta_2 \sin \theta_1, \]
\[ t_2 = \sin \theta_2 \sin \theta_1, \]
\[ t_3 = \sin \theta_3 \cos \theta_2, \]
\[ t_4 = \cos \theta_3 \cos \theta_1. \]

The case of \( N = 4J + 4 \) is similar to \( N = 4J + 2 \), and we present the two cases only, just for the sake of presentation: \((\theta_2, \theta_3) = (\frac{1}{8} \pi, \frac{3}{8} \pi)\) in Fig. 9 and \((\theta_2, \theta_3) = (\frac{1}{8} \pi, \frac{3}{8} \pi)\) in Fig. 10.

Edges phases are usually characterized by certain topological invariants. In 2D lattices these can be constructed in terms of \((A_\alpha, B_\alpha)\) instead of \((A_\alpha^+ \partial_x, B_\alpha^+ \partial_y)\) in Fig. 9 and \((A_\alpha^\pm, B_\alpha^\pm)\) in Fig. 10. This drawback can be overcome by introducing the Berry connections logical invariants. In 2D lattices these can be constructed in terms of \((A_\alpha, B_\alpha)\) instead of \((A_\alpha^+ \partial_x, B_\alpha^+ \partial_y)\) in Fig. 9 and \((A_\alpha^\pm, B_\alpha^\pm)\) in Fig. 10.

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4. Topological Invariants

Consider the tight-binding Hamiltonian

\[ H = \sum_n t_n (e^{i \epsilon_{n+1} e_n} + h.c.) \]

where \( t_n \) are periodic \( t_{n+2} = t_n \) and can be presented as

\[ t_n = \frac{1}{2} (t_1 + t_2) \cos \pi n. \]

Introduce the parameter \( \alpha \) by generalizing \( t_n \) as

\[ t_n - \alpha = \frac{1}{2} (t_1 + t_2) \cos \pi n + \alpha. \]

For \( \alpha = 0 \) we have \( t_{1,2} = t_{1,2} \), and \( t_{1,2} = t_{2,1} \) what represents the redefinition of a unit cell \( t_1 \rightarrow t_2 \). Increasing \( \alpha \) up to \( 2\pi \) we return back to \( t_{1,2} = t_{1,2} \). This construction is trivially extendable to any 1D periodic chain.

Rewriting (44) in the Fourier form, the corresponding one-particle Hamiltonian appears as

\[ \mathcal{H} = \begin{pmatrix}
0 & \tau_1 e^{ik} + \tau_2 e^{-ik}
\tau_1 e^{-ik} + \tau_2 e^{ik} & 0
\end{pmatrix}. \]

where \( \ell \) is the separation between the neighbouring sites, i.e. \( 2\ell \) is the period of the chain. In what follows we use the dimensionless momentum \( k \equiv (2\ell)k \) with \( -\pi \leq k \leq \pi \).

Eigenvalues and normalized eigenvectors are given by

\[ \epsilon^2(k, \alpha) = \tau_1^2 + \tau_2^2 + 2 \tau_1 \tau_2 \cos k, \]
\[ \psi(k, \alpha) = \frac{1}{\sqrt{2\epsilon^2}} \begin{pmatrix}
\tau_1 e^{i/2} + \tau_2 e^{-i/2}
\tau_1 e^{-i/2} + \tau_2 e^{i/2}
\end{pmatrix}. \]

hence the system is defined on a torus \( k \in [0,2\pi), \alpha \in [0,2\pi] \) depicted in Fig. 11.

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Introduce the parameter \( \alpha \) by generalizing \( t_n \) as

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For \( \alpha = 0 \) we have \( t_{1,2} = t_{1,2} \), and \( t_{1,2} = t_{2,1} \) what represents the redefinition of a unit cell \( t_1 \rightarrow t_2 \). Increasing \( \alpha \) up to \( 2\pi \) we return back to \( t_{1,2} = t_{1,2} \). This construction is trivially extendable to any 1D periodic chain.

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\tau_1 e^{-ik} + \tau_2 e^{ik} & 0
\end{pmatrix}. \]

where \( \ell \) is the separation between the neighbouring sites, i.e. \( 2\ell \) is the period of the chain. In what follows we use the dimensionless momentum \( k \equiv (2\ell)k \) with \( -\pi \leq k \leq \pi \).

Eigenvalues and normalized eigenvectors are given by

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\tau_1 e^{i/2} + \tau_2 e^{-i/2}
\tau_1 e^{-i/2} + \tau_2 e^{i/2}
\end{pmatrix}. \]

hence the system is defined on a torus \( k \in [0,2\pi), \alpha \in [0,2\pi] \) depicted in Fig. 11.
and the gauge invariant curvature is constructed as
\[ F = \partial_x A_y - \partial_y A_x. \] (50)

Let \( \Omega \) be the surface on the torus bounded by two closed contours corresponding to some \( \alpha_{1,2} \) as shown in Fig. 12.

Integrating the curvature (50) over \( \Omega \) and using Stokes' theorem we find
\[ \mu = \oint \mathbf{F} \cdot d\alpha = \oint A_x(x, \alpha_1) \, dx - \oint A_x(x, \alpha_2) \, dx \] (51)

where the right hand side represents the gauge invariant quantity referred to as the Zak phase.

Employing (48) we find
\[ A_x(x, \alpha) = \frac{1}{4\pi} \left( \tau_2 - \tau_1 \right) \cos \kappa \] (52)

Using this in (51) with \( \alpha_1 = 0 \) and \( \alpha_2 = \pi \) we find
\[ \mu = \text{sgn} \left( \tau_2 - \tau_1 \right) \] (53)

i.e. the Zak phase takes the values \( \pm 1 \).

### 4.2. Four-Band Chain

Consider now the Hamiltonian (44) with \( \alpha \)-dependent hopping parameters given by
\[ \tau_n = \frac{1}{4} \left( t_1 + t_2 + t_3 + t_4 - t_1 - t_2 + t_3 - t_4 \cos(\pi n + 2\alpha) + + \frac{3}{4}(t_1 - t_3) \sin(\frac{\pi n}{2} + \alpha) - \frac{1}{4}(t_2 - t_4) \cos(\frac{\pi n}{2} + \alpha) \right) \] (54)

with \( \tau_{n+4}(\alpha) = \tau_n(\alpha) \) and \( \tau_{n+2}(\alpha + 2\pi) = \tau_n(\alpha) \).

From (54) we find \( \tau_n(\alpha + 2\pi) = \tau_{n+4}(\alpha) \), meaning that the shift \( \alpha \rightarrow \alpha + 2\pi \) corresponds to the cyclic permutation \( t_1 \rightarrow t_2 \rightarrow t_3 \rightarrow t_4 \rightarrow t_1 \), hence the parameter \( \alpha \) introduced by (54) performs the interpolation between the different choices of elementary cells in the chain.

The corresponding one-particle Hamiltonian is given by
\[ H = \begin{pmatrix}
 0 & \tau_1 e^{i(4/4)\kappa} & 0 & \tau_4 e^{-i(4/4)\kappa} \\
\tau_1 e^{-i(4/4)\kappa} & 0 & \tau_2 e^{i(4/4)\kappa} & 0 \\
0 & \tau_2 e^{-i(4/4)\kappa} & 0 & \tau_3 e^{i(4/4)\kappa} \\
\tau_4 e^{i(4/4)\kappa} & 0 & \tau_3 e^{-i(4/4)\kappa} & 0
\end{pmatrix} \] (55)

where \( \kappa = (4\ell)k \) with \( 4\ell \) the chain period and \( -\pi \leq \kappa \leq +\pi \).

The four eigenvalues are given by
\[ 2\kappa^2(\kappa) = \tau_1^2 + \tau_2^2 + \tau_3^2 + \tau_4^2 \pm \sqrt{\tau_1^2 + \tau_2^2 + \tau_3^2 + \tau_4^2 + 4\tau_2^2 \tau_3 \tau_4}, \] (56)

where
\[ \kappa = (\tau_1^2 + \tau_2^2 + \tau_3^2 + \tau_4^2 - 4\tau_1^2 \tau_3 - 4\tau_2^2 \tau_4), \] (57a)
\[ \nu = 8\tau_1 \tau_2 \tau_3 \tau_4, \] (57b)

and are depicted in Fig. 13.

The spectrum is symmetric with respect to \( \epsilon \rightarrow -\epsilon \) since the Hamiltonian (55) enjoys the chiral symmetry.

Normalized eigenvectors \( (s = 1, 2, 3, 4) \) are given by
\[ \psi_s = \frac{1}{\sqrt{N_s}} \begin{pmatrix}
 c_1 \tau_1 e^{i(1/2)\kappa} + c_3 \tau_3 e^{-i(1/2)\kappa} \\
 c_2 (\tau_2^2 - \tau_4^2) e^{i(1/4)\kappa} + c_4 \tau_2 \tau_4 e^{-i(3/4)\kappa} \\
 c_3 (\tau_2^2 - \tau_4^2) e^{-i(3/4)\kappa} + c_1 \tau_2 \tau_4 e^{i(3/4)\kappa} \\
 c_2 \tau_2 \tau_4 e^{i(1/4)\kappa} + c_3 (\tau_2^2 - \tau_4^2)
\end{pmatrix} \] (58)

where \( N_s = 2c_1^2(\tau_1^2 - \tau_4^2)(\tau_2^2 - \tau_4^2)(\tau_3^2 - \tau_1^2)(\tau_4^2 - \tau_1^2)(\tau_1^2 + \tau_2^2 - \tau_3^2 - \tau_4^2) > 0 \).

Expressions (49) – (51) can be employed without any modification. Consequently, in order to obtain the gauge invariant topological indices we only need the expression for \( A_x(\kappa, \alpha) \). Using (58) in (49a) and performing trivial but lengthy manipulations we come to
\[ A_x^\pm(\kappa, \alpha) \equiv \oint A_x^\pm(\kappa, \alpha) \, d\kappa = \frac{1}{8\pi} \text{sgn}(\tau_2^2 - \tau_4^2) - \frac{1}{8\pi} \text{sgn}(\tau_1^2 - \tau_4^2) - \frac{1}{8\pi} \text{sgn}(\tau_1^2 - \tau_3^2) - \frac{1}{8\pi} \text{sgn}(\tau_2^2 - \tau_3^2), \] (59)

where
\[ \tau_n = \frac{1}{4} \left( t_1 + t_2 + t_3 + t_4 - t_1 - t_2 + t_3 - t_4 \cos(\pi n + 2\alpha) + + \frac{3}{4}(t_1 - t_3) \sin(\frac{\pi n}{2} + \alpha) - \frac{1}{4}(t_2 - t_4) \cos(\frac{\pi n}{2} + \alpha) \right) \] (60a)
\[ 4\pi C_1 = \frac{\tau_1^2 - \tau_2^2 - \tau_3^2 - \tau_4^2}{\tau_1^2 + \tau_2^2 + \tau_3^2 + \tau_4^2}, \] (60b)
\[ 2\pi C_2 = \frac{\tau_2^2 - \tau_3^2 - \tau_4^2}{\tau_1^2 + \tau_2^2 + \tau_3^2 + \tau_4^2}, \] (60c)
\[ 8\pi C_3 = \frac{(\tau_1^2 - \tau_2^2 - \tau_3^2 + \tau_4^2)(\tau_1^2 + \tau_2^2 - \tau_3^2 - \tau_4^2)}{\tau_1^2 + \tau_2^2 + \tau_3^2 + \tau_4^2}. \] (60c)

Mind that the connection (59) involves \( \epsilon^2 \) rather than \( \epsilon \). Using (56) and integrating over \( \kappa \) we obtain
\[ \mu_\pm(\alpha) \equiv \oint A_x^\pm(\kappa, \alpha) \, d\kappa = \frac{1}{2\pi} \frac{1}{u + v} \] (61)
where $K$ and $\Pi$ are the complete elliptic integrals

$$K(x) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-x^2 \sin^2 \theta}},$$

$$\Pi(y,x) = \int_0^{\pi/2} \frac{d\theta}{(1-y^2 \sin^2 \theta)\sqrt{1-x^2 \sin^2 \theta}},$$

and

$$\lambda = \frac{4t_1t_2t_3}{(t_1t_3 - t_2t_4)^2},$$

$$\zeta = \frac{4t_1t_2t_3}{(t_1t_2 + t_3t_4)^2}.$$

If the system is quarter-filled we employ $\mu_+(\alpha)$ corresponding to the lowest band $\epsilon = -\epsilon_+$ in Fig. 13. We then search for the combinations $\mu_+(\alpha_1) - \mu_+(\alpha_2)$ which (besides being gauge invariants) would be quantized. Taking into account that the last three terms of (61) are insensitive to $\alpha \to \alpha + \pi$, we find that the sought for quantization occurs for $|\alpha_1 - \alpha_2| = \pi$. In particular, we find

$$\sigma_2 \equiv \text{sgn}(t_1^2 t_2^2 - t_2^2 t_4^2) = \mu_+(\frac{\pi}{2}) - \mu_+(\frac{3\pi}{2}),$$

$$\sigma_3 \equiv \text{sgn}(t_1^2 t_2^2 - t_3^2 t_4^2) = \mu_+(\pi) - \mu_+(0).$$

These parameters are responsible for splitting off certain edge state levels from the lowest band, e.g., $\epsilon = -(t_1^2 + t_2^2)^{1/2}$ and $\epsilon = -(t_1^2 + t_3^2)^{1/2}$ splitting off the lowest band in Fig. 6. Remark that $\sigma_1 \equiv \text{sgn}(t_1 t_3 - |t_2 t_4|)$ does not emerge here. This is reasonable since $\sigma_1$ controls closing/opening of the central gap (it is closed for $t_1 t_3 = t_2 t_4$), which is irrelevant due to the quarter-filling.

For half-filling we sum up over the two lower bands. In that case we trivially come to

$$\mu(\alpha) \equiv \mu_+(\alpha) + \mu_-(\alpha) =$$

$$= \frac{1}{2} \text{sgn}(|t_1 t_3| - |t_2 t_4|) - \text{sgn}(|t_1 t_2| - |t_3 t_4|)$$

where from the parameters $\sigma_{1,2,3}$ can be expressed as

$$\sigma_1 \equiv \text{sgn}(t_1^2 t_3^2 - t_2^2 t_4^2) = \mu(0) - \mu(\frac{\pi}{2}) + \mu(\frac{\pi}{2}),$$

$$\sigma_2 \equiv \text{sgn}(t_1^2 t_2^2 - t_3^2 t_4^2) = \mu(\frac{\pi}{2}) - \mu(\frac{3\pi}{2}),$$

$$\sigma_3 \equiv \text{sgn}(t_1^2 t_2^2 - t_3^2 t_4^2) = \mu(\pi) - \mu(0).$$

Remark that the three combinations standing in the right hand sides of (66) are linearly independent.

5. Conclusions

Summarizing, we have studied the issue of edge states in a tight-binding model on a finite chain with four-fold alternated hoppings. Employing the technique developed in Ref. [7], the one-particle eigenvalue problem is solved analytically and the wave functions are expressed in terms of the Chebyshev polynomials $U_n(x)$. Energy eigenvalues of the edge states and the conditions for their formation are also found analytically. All analytic results are confirmed by numeric calculations.

It is found that the chains with odd number of sites produce 4 phases which differ one from another with respect to the content (presence/absence) of various edge states, while chains with even sites produce 8 different phases.

Remark also that the flat shapes of some edge state levels result from particular parameterizations. To be clear we present the phase diagramme for $N = \text{odd}$ in Fig. 14.

Figs. 2, 3 and 4 depict the energy spectra $\epsilon_{1-101}$ versus the parameter $\theta_1$ introduced by (30). Varying $\theta_1$ we thus vary the ratio $t_1/t_2$ while $t_3/t_4$ is kept constant. This corresponds to the dashed straight lines shown in Fig. 14; the lowest corresponds to $\theta_2 < \frac{3\pi}{4}$ where the phase C isolates A from D; middle one is for $\theta_2 = \frac{3\pi}{4}$, so that no intermediate phase occurs between A and D; and the upper one is for $\theta_2 > \frac{3\pi}{4}$ with A and D separated by B. In these three cases the edge state levels (Figs. 2,3,4) are all flat.

Alternatively, one may plot the spectrum $\epsilon_{101}$ versus the parameter varying along the circular path in Fig. 14. In that case the spectrum looks as in Fig. 15 and the edge state energy levels $\epsilon = \pm(t_1^2 + t_3^2)^{1/2}$ and $\epsilon = \pm(t_2^2 + t_4^2)^{1/2}$ are no longer flat but interpolate between the two bands.

Further, we have proposed the scheme for constructing gauge invariant curvature applicable to general 1D periodic chain. In the case of the two-band model the scheme reproduces the Zak phase, while for the four-band model...
it recovers the defining parameters $\sigma_{1,2,3}$ as gauge invariant topological indices.

As previously pointed out, the shift $a \rightarrow a + \frac{1}{4}\pi$ in $\tau_n(a)$ represents the permutation $t_1 \rightarrow t_2 \rightarrow t_3 \rightarrow t_4 \rightarrow t_1$ which can be treated as translation of the chain in $x$-space, while the shift of $\kappa$ represents translation in momentum space. In this light the pair $(\kappa, a)$ resembles canonical conjugate pair, while the torus might be regarded as the corresponding phase space.

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Appendix A: Three-Term Periodic Recursion

We solve the recurrence relation

$$t_n \psi_n + \epsilon \psi_{n+1} + t_{n+1} \psi_{n+2} = 0$$

(A1)

provided the coefficients are periodic $t_{n+\omega} = t_n$.

For this purpose we employ the results of Ref. [7]. Let $p_n(x)$ be a sequence of polynomials set by the recursion

$$p_n(x) = (x + b_{n-1})p_{n-1}(x) - a_{n-1}p_{n-2}(x)$$

(A2)

supplied by the boundary conditions $p_{-1} = 0$ and $p_0 = 1$, and the periodic coefficients $a_{n+\omega} = a_n$ and $b_{n+\omega} = b_n$.

As shown in Ref. [7] the polynomial $p_{n+\omega}$ divides $p_{2n-1}$

$$q(x) = \frac{p_{2n-1}(x)}{p_{n+1}(x)}$$

(A3)

where $q(x)$ is of order of $\omega$.

Then the solution to (A2) appears as

$$p_{n+\omega} = a^{n-1}p_{\omega \omega}U_{n-1}(q/2a) - a^n p_{\omega}U_{n-2}(q/2a)$$

(A4)

where $a^\omega = a_{12}a_{13}...a_{\omega}$.

We proceed to bring (A1) to the form (A2). Introducing $p_n = (t_1...t_n) \psi_{n+1}$ we rewrite (A1) as

$$p_{n+1} = -\epsilon p_n - t_n^2 p_{n-1}$$

(A5)

and the boundary condition $\psi_{\omega} = 0$ takes the form $p_{-1} = 0$.

We thus come to the recursion set by (A2) with $a_n = t_n^2$ and $b_n = 0$.

For the two-band model the periodicity is $\omega = 2$, and $q(\epsilon)$ set by (A3) appears as

$$q(\epsilon) = \epsilon^2 - t_1^2 - t_2^2.$$  

(A6)

Using (A4) we solve $p_n$ and rewriting in terms of $\psi_n$ find

$$\psi_{2n+2}(\epsilon) = \psi_{s+2}(\epsilon)U_{n-1}(\xi) - \psi_{s}(\epsilon)U_{n-2}(\xi),$$

(A7)

where

$$\xi = \frac{\epsilon^2 - t_1^2 - t_2^2}{2t_1t_2}.$$  

(A8)

Writing out (A7) for $s = 1, 2$ we find

$$\psi_{2n+1} = \psi_{3U_{n-1}(\xi)} - \psi_{1U_{n-2}(\xi)},$$

(A9a)

$$\psi_{2n+2} = \psi_{4U_{n-1}(\xi)} - \psi_{2U_{n-2}(\xi)}.$$  

(A9b)

Employing the recursion (A1) we express $\psi_{2,3,4}$ in terms of $\psi_1$ and rewrite (A9) as (4).

For the four-band model the periodicity is $\omega = 4$, and $q(\epsilon)$ set by (A3) appears as

$$q(\epsilon) = \epsilon^4 - \left( t_1^2 + t_2^2 + t_3^2 + t_4^2 \right)^2 + \left( t_1^2 t_3^2 + t_2^2 t_4^2 \right)$$  

(A10)

Using (A4) we solve $p_n$ and rewriting in terms of $\psi_n$ find

$$\psi_{4n+2}(\epsilon) = \psi_{s+4}(\epsilon)U_{n-1}(\xi) - \psi_{s}(\epsilon)U_{n-2}(\xi),$$

(A11)

where

$$\xi = \frac{\epsilon^4 - (t_1^2 + t_2^2 + t_3^2 + t_4^2)^2 + t_1^2 t_3^2 + t_2^2 t_4^2}{2t_1t_2t_3t_4}.$$  

(A12)

Writing out (A11) for $s = 1, 2, 3, 4$ we find

$$\psi_{4n+1} = \psi_{5U_{n-1}(\xi)} - \psi_{1U_{n-2}(\xi)},$$

(A13a)

$$\psi_{4n+2} = \psi_{6U_{n-1}(\xi)} - \psi_{2U_{n-2}(\xi)},$$

(A13b)

$$\psi_{4n+3} = \psi_{7U_{n-1}(\xi)} - \psi_{3U_{n-2}(\xi)},$$

(A13c)

$$\psi_{4n+4} = \psi_{8U_{n-1}(\xi)} - \psi_{4U_{n-2}(\xi)}.$$  

(A13d)

Employing (A1) we express $\psi_{2,8}$ via $\psi_1$ and rewrite (A13) as (22). In so doing we use $U_{n+1}(x) = 2xU_n(x) - U_{n-1}(x)$.

Appendix B: $N = 4J + 1$

We search for the edge states provided $J \to \infty$. For this purpose we study the equation (26a)

$$\epsilon \left[ \frac{U_J(\xi)}{U_{J-1}(\xi)} + \frac{t_1t_4}{t_2t_3} \right] = 0.$$  

(B1)

Since the edge states emerge only when $|\xi| > 1$, we analyze the equation (B1) for $\xi > 1$ and $\xi < -1$.

For $\xi > 1$. In this case we have $U_J(\xi) > 0$, hence the only solution to (B1) is given by $\epsilon = 0$. Using this in (23) we find

$$\xi = \frac{1}{2} \left( \frac{t_1t_3}{t_2t_4} - \frac{t_2t_3}{t_1t_4} \right) > 1.$$  

(B2)

i.e. we have $\xi > 1$ except when $t_1t_3 = t_2t_4$ where $\xi = 1$.  

We are now about to use (B2) in (22) and (25) involving the quantities \( U_n(\xi) \). Here we use the relation

\[
U_n \left[ \frac{1}{2} \left( x + \frac{1}{x} \right) \right] = \frac{1 - x^{2n+2}}{x^n(1-x^2)} \tag{B3}
\]

which in fact is the same (10) and allows to calculate \( U_n(\xi) \) in the exact way. For \( t_1 t_3 < t_2 t_4 \) we use (22) and come to (27), while for \( t_1 t_3 > t_2 t_4 \) we use (25) and come to (28).

\[ \xi < -1. \]  
In this case we put \( \xi = -\cosh z \) and using (10) write the ratio of two polynomials standing in (B1) as

\[
\frac{U_J(\xi)}{U_{J-1}(\xi)} = \frac{\sinh[(J+1)z]}{\sinh[Jz]} \tag{B4}
\]

Taking \( J \to \infty \) we put \( z > 0 \) (the same final result occurs for \( z < 0 \)) and come to

\[
\frac{U_J(\xi)}{U_{J-1}(\xi)} \to -e^z. \tag{B5}
\]

Using this in (B1) we obtain

\[
e^z = \frac{t_1 t_4}{t_2 t_3}. \tag{B6}
\]

Provided \( z \) is taken to be positive, the last relation implies that the case under consideration can be realized only if \( t_1 t_4 > t_2 t_3 \).

Substituting (B6) into \( \xi = -\cosh z \) we rewrite the equation (23) as \( (e^2 - t_1^2 - t_2^2)(e^2 - t_3^2 - t_4^2) = 0 \) producing four levels

\[
e = \pm(t_1^2 + t_2^2)^{1/2}, \tag{B7a}
\]

\[
e = \pm(t_3^2 + t_4^2)^{1/2}. \tag{B7b}
\]

For (B7a) we use (22) and come to (29a), while for (B7b) we use (25) and come to (29b).

**Appendix C: \( N = 4J + 3 \)**

We study the secular equation (26b) in the limit of \( J \to \infty \) and consider the cases \( |\xi| > 1 \).

\[ \xi > 1. \]  
Taking \( \xi = \cosh z \) we write the equation (26b) as

\[
e^2 - t_1^2 = \frac{\sinh[(J+1)z]}{\sinh[Jz]} + \frac{t_4}{t_3} \tag{C1}
\]

Assuming \( z > 0 \), and taking the limit \( J \to \infty \) this leads to

\[
e^2 = \frac{t_4}{t_3} \frac{t_1 t_2}{t_2^2 - t_1^2}. \tag{C2}
\]

Substituting (C2) into \( \xi = \cosh z \) and combining with (23) we come up to the following three equations

\[
e^2 = 0, \tag{C3a}
\]

\[
e^2 = t_1^2 + t_2^2, \tag{C3b}
\]

\[
e^2 = t_3^2 + t_4^2. \tag{C3c}
\]

Last two options are controversial since the right hand side of (C2) becomes negative. Using (C3a) in (C2) we find

\[
e^2 = \frac{t_2 t_4}{t_1 t_3}, \tag{C4}
\]

i.e. provided \( z > 0 \), we may have \( \xi > 1 \) only for \( t_1 t_3 < t_2 t_4 \) with \( e^2 = 0 \). The fact that the eigenvalue occurs as \( e^2 = 0 \) signifies the energy level with \( e = 0 \) is doubly degenerated. One of the two wave functions is obtained by assuming \( \psi_1 \) is finite. In that case we use (22) and come to (31a). The other is obtained by assuming \( \psi_N \) is finite. In that case we use (25) which leads to (31b).

\[ \xi < -1. \]  
We put \( \xi = -\cosh z \) and rewrite the equation (23) as

\[
e^2 - t_1^2 = \frac{\sinh[(J+1)z]}{\sinh[Jz]} \frac{t_4}{t_3} = 0 \tag{C5}
\]

Assuming \( z > 0 \), and taking the limit \( J \to \infty \) we obtain

\[
e^2 = \frac{t_4}{t_3} \frac{t_1 t_2}{t_2^2 - t_1^2}. \tag{C6}
\]

Substituting this into \( \xi = -\cosh z \) and combining with (23) we come to the same three options given by (C3). In this case the first option is controversial and we study the last two

\[
e^2 = t_1^2 + t_2^2 \quad \Rightarrow \quad e^2 = t_1 t_4/t_2 t_3, \tag{C7a}
\]

\[
e^2 = t_1^2 + t_4^2 \quad \Rightarrow \quad e^2 = t_1 t_2/t_3 t_4. \tag{C7b}
\]

which may occur for \( t_1 t_4 > t_2 t_3 \) and \( t_1 t_2 > t_3 t_4 \), respectively.

For (C7a) we use (22) and come to (32). For (C7b) we use (25) which gives (33).

**Appendix D: \( N = 4J + 3 \)**

Secular equation (26c) breaks into the following three

\[
c = 0, \tag{D1a}
\]

\[
e^2 = t_1^2 + t_2^2, \tag{D1b}
\]

\[
U_J(\xi) = 0. \tag{D1c}
\]

The roots of Chebyshev polynomials are all located in the segment \((-1,1)\), hence (D1c) leads to \( |\xi| < 1 \), i.e. to bulk states.

**Using \( c = 0 \) in (23)** we find \( \xi = \frac{1}{2}(t_1 t_3/t_2 t_4) + \frac{1}{2}(t_2 t_4/t_1 t_3) \) and we consider the two options \( t_1 t_3 < t_2 t_4 \) and \( t_1 t_3 > t_2 t_4 \). In the first case we use (22) and come to (34), while for the other we use (25) and come to (35).

**Using \( e^2 = t_1^2 + t_2^2 \) in (23)** we obtain

\[
\xi = \frac{t_1^2 t_2^2 + t_1^2 t_4^2}{2 t_1 t_2 t_3 t_4} \leq -1 \tag{D2}
\]

and we have two options \( t_1 t_4 > t_2 t_3 \) and \( t_1 t_4 > t_2 t_4 \). In the first case we use (22) and come to (36). For the other we use (25) and come to (37).


Appendix E: $N = 4J + 4$

\[\dot{\xi} > 1.\] Taking $\xi = \cosh z$ the equation (26d) reads

\[
\frac{\sinh[(J+2)z]}{\sinh[(J+1)z]} + \frac{t_4 \epsilon^2 - t_2^2}{t_3 \ t_1 t_2} = 0. \tag{E1}
\]

Assuming $z > 0$ we take the limit $J \to \infty$ and obtain

\[
e^z = -\frac{t_4 \epsilon^2 - t_2^2}{t_3 \ t_1 t_2}. \tag{E2}
\]

Using this in $\xi = \cosh z$ and combining with (23) we find

\[e^z = 0, \tag{E3a}\]
\[e^z = t_1^2 + t_2^2, \tag{E3b}\]
\[e^z = t_2^2 + t_3^2. \tag{E3c}\]

(E3b) and (E3c) controversial since the right hand side of (E2) becomes negative. Using (E3a) in (E2) we find

\[
e^z = \frac{t_2 t_4}{t_1 t_3}, \tag{E4}
\]

i.e. provided $z > 0$, we may have $\dot{\xi} > 1$ only if $t_1 t_3 < t_2 t_4$ with $\epsilon^2 = 0$. The fact that the eigenvalue occurs as $\epsilon^2 = 0$ implies the energy level with $\epsilon = 0$ is doubly degenerated. One of the two is obtained using (22) and leads to (38a). The other one is obtained using (25) and appears as (38b).

\[\dot{\xi} < -1.\] Taking $\xi = -\cosh z$, the secular equation (26d) reads

\[
\frac{\sinh[(J+2)z]}{\sinh[(J+1)z]} - \frac{t_4 \epsilon^2 - t_2^2}{t_3 \ t_1 t_2} = 0. \tag{E5}
\]

Assuming $z > 0$, and taking the limit $J \to \infty$ we obtain

\[
e^z = \frac{t_4 \epsilon^2 - t_2^2}{t_3 \ t_1 t_2}. \tag{E6}
\]

Substituting this into $\xi = -\cosh z$ and combining with (23), we obtain the same three options (E3). First option is controversial, and we study the last two ones

\[e^z = \frac{t_4 \epsilon^2 - t_2^2}{t_3 \ t_1 t_2} \implies e^z = \frac{t_1 t_4}{t_2 t_3}, \tag{E7a}\]
\[e^z = \frac{t_4 \epsilon^2 - t_2^2}{t_3 \ t_1 t_2} \implies e^z = \frac{t_3 t_4}{t_1 t_2}, \tag{E7b}\]

hence the first one occurs if $t_1 t_4 > t_2 t_3$, and the second one occurs for $t_1 t_4 < t_2 t_3$. In the first case we use (22) find (39), while in the second one we use (25) and come to (40).

[1] B. A. Bernevig, T. L. Hughes, Topological Insulators and Topological Superconductors (Princeton Univ. Press, 2013).
[2] S.-Q. Shen, Topological Insulators (Springer, 2012).
[3] J. K. Asbóth, L. Oroszlány, A. Pályi, A Short Course on Topological Insulators (Springer, 2016).
[4] W. P. Su, J. R. Schrieffer, A. J. Heeger, Phys. Rev. Lett. 42, 1698 (1979).
[5] Linhu Li, Zhihao Xu, Shu Chen, Phys. Rev. B 89, 085111 (2014).
[6] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
[7] B. Beckermann, J. Gilewicz, E. Leopold, Appl. Math. 23, 319 (1995).
[8] J. Zak, Phys. Rev. Lett. 62, 2747 (1989).
[9] M. Eliashvili, G. I. Japaridze, G. Tsitsishvili, G. Tukhashvili, J. Phys. Soc. Jpn. 83, 044706 (2014).
[10] S. Mao, Y. Kuramoto, K.-I. Imura, A. Yamakage, J. Phys. Soc. Jpn. 79, 124709 (2010).
[11] E. H. Lieb, Phys. Rev. Lett. 62, 1201 (1989).
[12] T. Kariyado, Y. Hatsugai, Phys. Rev. B 90, 085132 (2014).