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TOPOLOGICAL PHASES IN 2D TIGHT-BINDING MODEL ON A RIBBON

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Abstract. We analyze the formation of edge and bulk states on a lattice ribbon in the framework of a tight-binding model. We show that three different phases may develop. These are genuine edge states, genuine bulk states and the phase where the bulk and edge states coexist.

1. Introduction

The main imprint of topological order in two-dimensional electron systems is the occurrence of edge states [2]. The physics of edge states has become the subject of intense studies due to the progress in fabrication of low-dimensional electron structures where the phases of matter are described in terms of topological concepts rather than in term of symmetries [3]. The common picture for studying such systems is based on tight-binding models (e.g., [1]) of various geometric configurations with and/or without boundaries. In this paper, we consider a tight-binding model of free electrons living on a two-dimensional lattice ribbon. Electron delocalization is characterized by four nearest neighbor hopping parameters. The simplified version of this model has been studied in [4] where the eigenvalue equation is reduced to a three-term recurrence relation by turning off one of the four hopping parameters. In that case, the occurrence of edge and bulk states has been described in the exact analytic form in terms of the Chebyshev polynomials. In the present account, we keep all four parameters leading to a five-term recurrence relation and resulting in the possibility of three different phases: 1) simultaneous occurrence of two edge states with different length scales; 2) simultaneous occurrence of two bulk states with different oscillation lengths; and 3) coexistence of one edge and one bulk state.

2. The Model

We study the tight-binding model on a ribbon shown in Figure 1.

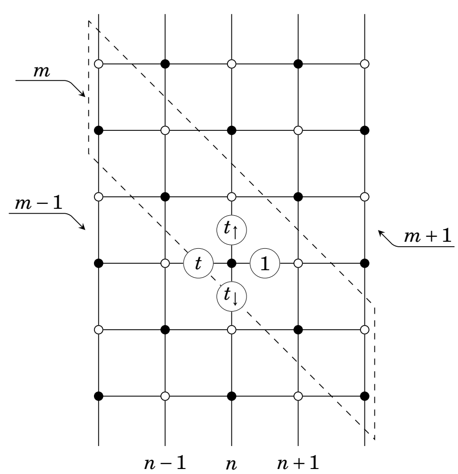

Figure 1

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The corresponding tight-binding Hamiltonian appears as

$$
\begin{aligned}
H = t_\uparrow \sum_m \sum_{n=1}^{N} \Big[c_\circ^\dagger(n,m) c_\bullet(n,m) + h.c.\Big] + t_\downarrow \sum_m \sum_{n=1}^{N} \Big[c_\circ^\dagger(n,m-1) c_\bullet(n,m) + h.c.\Big] \\
+ t \sum_m \sum_{n=2}^{N} \Big[c_\circ^\dagger(n-1,m-1) c_\bullet(n,m) + h.c.\Big] + \sum_m \sum_{n=1}^{N-1} \Big[c_\circ^\dagger(n+1,m) c_\bullet(n,m) + h.c.\Big]
\end{aligned}
\tag{2.1}
$$

describing the hoppings of electrons between the nearest neighbouring sites. Hopping parameter in the last term is scaled to one, while the rest of the parameters are denoted by $t_\uparrow, t_\downarrow, t$. Performing the Fourier transform ($\mu = \bullet, \circ$)

$$
c_\mu(n,m) = \frac{1}{\sqrt{2\pi}} \oint e^{+ikm} c_{\mu n}(k) dk \tag{2.2}
$$

and introducing the notation $C_\mu(k) = \big(c_{\mu 1}(k), \ldots, c_{\mu N}(k)\big)^T$, we rewrite (2.1) in the following form:

$$
H = \oint \Big(C_\bullet^\dagger, C_\circ^\dagger\Big) \begin{pmatrix} 0 & T^\dagger \\ T & 0 \end{pmatrix} \begin{pmatrix} C_\bullet \\ C_\circ \end{pmatrix} dk, \tag{2.3}
$$

where

$$
T = t_\uparrow + t_\downarrow e^{+ik} + t e^{+ik} \beta^\dagger + \beta \tag{2.4a}
$$

$$
\beta = \begin{pmatrix}
0 & 0 & 0 & \cdots & 0 & 0 \\
\mathbf{1} & 0 & 0 & \cdots & 0 & 0 \\
0 & \mathbf{1} & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & \cdots & \mathbf{1} & 0
\end{pmatrix} . \tag{2.4b}
$$

The occurrence of edge and bulk states can be described in terms of the eigenstates of the one-particle Hamiltonian standing in the integrand of (2.3). Therefore we study the eigenvalue problem

$$
\begin{pmatrix} 0 & T^\dagger \\ T & 0 \end{pmatrix} \begin{pmatrix} \psi_\bullet \\ \psi_\circ \end{pmatrix} = \mathcal{E} \begin{pmatrix} \psi_\bullet \\ \psi_\circ \end{pmatrix} . \tag{2.5}
$$

We search for the solutions to (2.5) in the form $\psi_\mu = G\phi_\mu$, where $G = \mathrm{diag}\big(e^{-(i/2)k}, \ldots, e^{-N(i/2)k}\big)$. Using $G\beta^\dagger G^\dagger = e^{+(i/2)k}\beta^\dagger$ and $G\beta G^\dagger = e^{-(i/2)k}\beta$, we arrive at

$$
\begin{cases}
(t_\uparrow e^{-(i/2)k} + t_\downarrow e^{+(i/2)k} + \beta + t\beta^\dagger)\phi_\bullet = \mathcal{E} e^{-(i/2)k} \phi_\circ, \\
(t_\uparrow e^{+(i/2)k} + t_\downarrow e^{-(i/2)k} + \beta^\dagger + t\beta)\phi_\circ = \mathcal{E} e^{+(i/2)k} \phi_\bullet.
\end{cases} \tag{2.6}
$$

Eliminating ϕ_0, we obtain $\Omega_\bullet \phi_\bullet = \omega \phi_\bullet$, where $\Omega_\bullet$ is an $N \times N$ penta-diagonal matrix (if eliminating $\phi_\bullet$, one obtains $\Omega_\circ \phi_\circ = \omega \phi_\circ$, where $\Omega_\circ$ leads to the same eigenvalue problem)

$$
\Omega_\bullet = \begin{pmatrix}
-t^2 & \bar{w} & t & 0 & \cdots & 0 & 0 & 0 & 0 \\
w & 0 & \bar{w} & t & \cdots & 0 & 0 & 0 & 0 \\
t & w & 0 & \bar{w} & \cdots & 0 & 0 & 0 & 0 \\
0 & t & w & 0 & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 0 & \bar{w} & t & 0 \\
0 & 0 & 0 & 0 & \cdots & w & 0 & \bar{w} & t \\
0 & 0 & 0 & 0 & \cdots & t & w & 0 & \bar{w} \\
0 & 0 & 0 & 0 & \cdots & 0 & t & w & -1
\end{pmatrix} \tag{2.7}
$$

with

$$w = (1+t)u + i(1-t)v, \tag{2.8a}$$
$$u = (t_\uparrow + t_\downarrow)\cos(k/2), \tag{2.8b}$$
$$v = (t_\uparrow - t_\downarrow)\sin(k/2), \tag{2.8c}$$
$$\omega = \mathcal{E}^2 - u^2 - v^2 - 1 - t^2. \tag{2.8d}$$

Writing out $\Omega_\bullet \phi_\bullet = \omega\phi_\bullet$ in the component form, we obtain

$$t\phi_3 + \bar{w}\phi_2 - (\omega + t^2)\phi_1 = 0, \tag{2.9a}$$
$$t\phi_4 + \bar{w}\phi_3 - \omega\phi_2 + w\phi_1 = 0, \tag{2.9b}$$
$$t\phi_{n+2} + \bar{w}\phi_{n+1} - \omega\phi_n + w\phi_{n-1} + t\phi_{n-2} = 0, \qquad 3 \leqslant n \leqslant N-2, \tag{2.9c}$$
$$\bar{w}\phi_N - \omega\phi_{N-1} + w\phi_{N-2} + t\phi_{N-3} = 0, \tag{2.9d}$$
$$-(\omega+1)\phi_N + w\phi_{N-1} + t\phi_{N-2} = 0. \tag{2.9e}$$

We regard this system as the recurrence (2.9c) for general n with the rest four equations serving as the initial conditions. Searching for the solution to (2.9c), as $\phi_n = z^n$, we come to the quartic equation

$$tz^4 + \bar{w}z^3 - \omega z^2 + wz + t = 0. \tag{2.10}$$

So, the general solution to (2.9c) appears as

$$\phi_n = A_1 z_1^n + A_2 z_2^n + A_3 z_3^n + A_4 z_4^n, \tag{2.11}$$

where $z_{1,2,3,4}$ are the four (complex) roots of (2.10), and the constants $A_{1,2,3,4}$ have to be fixed by the initial conditions.

If z is the root of (2.10), then $1/\bar{z}$ is the root, as well. Besides, $z_1z_2z_3z_4 = 1$ as it follows from (2.10). Therefore we may have the following three cases for the set of the roots

$$\{z\} = \{r_1e^{+i\alpha}, r_2e^{-i\alpha}, (1/r_1)e^{+i\alpha}, (1/r_2)e^{-i\alpha}\}, \tag{2.12a}$$
$$\{z\} = \{r_1e^{+i\alpha}, e^{-i\alpha+i\alpha_2}, (1/r_1)e^{+i\alpha}, e^{-i\alpha-i\alpha_2}\}, \tag{2.12b}$$
$$\{z\} = \{e^{+i(\alpha+\alpha_1)}, e^{-i(\alpha-\alpha_2)}, e^{+i(\alpha-\alpha_1)}, e^{-i(\alpha+\alpha_2)}\}, \tag{2.12c}$$

where $|r_{1,2}| < 1$.

In the first case we have two edge states with the length scales $r_{1,2}$, *i.e.*, the factors $(r_{1,2})^n$ in (2.11) are localized at the left edge ($n = 0$), while $(1/r_{1,2})^n$ are localized at the right edge ($n = N$). In the second case, we have one edge state set by r_1 and one bulk state set by $e^{\pm i\alpha_2}$ oscillating with respect to n ($\phi_n \sim e^{\pm in\alpha_2}$). In the third case, we have two bulk states set by $e^{+i\alpha_1}$ and $e^{+i\alpha_2}$.

The main question we address is formulated as follows: which of the above three phases occurs depending on the input parameters $(t_\uparrow, t_\downarrow, t, k)$. A comprehensive analysis of this problem is technically complicated. Therefore we present the case of $v = 0$ as a demonstrative example of how the three phases (2.12) may occur for different settings.

3. The Case of $v = 0$

This case occurs either for $t_\uparrow = t_\downarrow$ or for $k = 0$. We have

$$u = \begin{cases} 2t_\uparrow \cos(k/2) & \text{for} \quad t_\uparrow = t_\downarrow \\ t_\uparrow + t_\downarrow & \text{for} \quad k = 0 \end{cases} \tag{3.1}$$

and the equation (2.10) breaks up into two quadratic equations

$$z + \frac{1}{z} = -\frac{1+t}{2t}u + \frac{1}{2t}\sqrt{(u^2-4t)(1-t)^2 + 4t\mathcal{E}^2}, \tag{3.2a}$$
$$z + \frac{1}{z} = -\frac{1+t}{2t}u - \frac{1}{2t}\sqrt{(u^2-4t)(1-t)^2 + 4t\mathcal{E}^2}, \tag{3.2b}$$

where (3.2a) and (3.2b) produce two solutions each for z.

For $(u^2 - 4t)(1-t)^2 + 4t\mathcal{E}^2 < 0$, the right-hand sides of (3.2) are complex, hence none of the four roots can be located on a unit circle (otherwise the left-hand sides are real), implying the occurrence of two edge states (2.12a). The roots are all complex and we have labelled this phase by E_c in the table below with E denoting "edge" and the subscript "c" indicating that the roots are complex.

For $(u^2-4t)(1-t)^2+4t\mathcal{E}^2>0$, the right-hand sides of (3.2) are real, hence $z+z^{-1}$ is real, as well. If $z+z^{-1}<-2$, then z is real negative. For $-2<z+z^{-1}<2$, we have $z=e^{i\alpha}$. For $z+z^{-1}>2$, the value of z is real positive. Therefore (3.2a) and (3.2b) each give the corresponding three options which we label as (❶,❷,❸) and (①,②,③) respectively. Thus we have

$$\text{(3.2a)} \Rightarrow \left.\begin{cases} ❶ \quad z_{1,2}<0 & \Rightarrow \quad -(1+t)u+\sqrt{(u^2-4t)(1-t)^2+4t\mathcal{E}^2}<-4t \\ ❷ \quad z_{1,2}=e^{i\gamma_{1,2}} & \Rightarrow \quad -4t<-(1+t)u+\sqrt{(u^2-4t)(1-t)^2+4t\mathcal{E}^2}<+4t \\ ❸ \quad z_{1,2}>0 & \Rightarrow \quad +4t<-(1+t)u+\sqrt{(u^2-4t)(1-t)^2+4t\mathcal{E}^2} \end{cases}\right\} \quad \text{(3.3a)}$$

$$\text{(3.2b)} \Rightarrow \left.\begin{cases} ① \quad z_{3,4}<0 & \Rightarrow \quad -(1+t)u-\sqrt{(u^2-4t)(1-t)^2+4t\mathcal{E}^2}<-4t \\ ② \quad z_{3,4}=e^{i\gamma_{3,4}} & \Rightarrow \quad -4t<-(1+t)u-\sqrt{(u^2-4t)(1-t)^2+4t\mathcal{E}^2}<+4t \\ ③ \quad z_{3,4}>0 & \Rightarrow \quad +4t<-(1+t)u-\sqrt{(u^2-4t)(1-t)^2+4t\mathcal{E}^2}, \end{cases}\right\} \quad \text{(3.3b)}$$

implying 9 different combinations. The option ❶ is incompatible with ② as well as with ③, while ❷ is incompatible with ③. The rest six combinations are itemized in the following table

Combinations	Label	Restrictions on u and $\mathcal{E}^2$	
❶①	E	$u>4t(1+t)^{-1}$	$\frac{1}{4}t^{-1}(4t-u^2)(1-t)^2<\mathcal{E}^2<(1+t-u)^2$
❷①	BE	$u>0$	$(1+t-u)^2<\mathcal{E}^2<(1+t+u)^2$
❷②	B	$\lvert u\rvert<4t(1+t)^{-1}$	$\frac{1}{4}t^{-1}(4t-u^2)(1-t)^2<\mathcal{E}^2<(1+t-\lvert u\rvert)^2$
❸①	$E_\pm$	$-\infty<u<+\infty$	$(1+t+\lvert u\rvert)^2<\mathcal{E}^2$
❸②	BE	$u<0$	$(1+t+u)^2<\mathcal{E}^2<(1+t-u)^2$
❸③	E	$u<-4t(1+t)^{-1}$	$\frac{1}{4}t^{-1}(4t-u^2)(1-t)^2<\mathcal{E}^2<(1+t+u)^2$

In the case of ❶①, the four roots are all real negative numbers. Then the factors of $(-1)^n$ arising from z^n in (2.11) become irrelevant, since they can be factorized out as an overall phase. Therefore the case of ❶① is equivalent to the one of ❸③, where the roots are all real positive. These correspond to (2.12a) implying two edge states. We have denoted such a phase as E.

In the case of ❷①, two roots are phases ($e^{\pm i\alpha}$) and the rest two are real negative. Provided the two roots are phases, the negativity/positivity of the rest two roots does not make any sense. Therefore this is equivalent to the case of ❸②. We denote these phases as BE implying the mixture of edge and bulk states (2.12b).

In the case of ❷②, all roots are phases meaning genuine bulk state (2.12c). We denote it as B.

In the case of ❸①, two roots are real positive, while the rest two are real negative implying the case of two edge states (2.12a) which, however, differs from E, since the factor of $(-1)^n$ occurring only in one pair of roots cannot be factorized out. Therefore we denote it as $E_\pm$.

Collecting all the described cases, we construct the phase diagramme where the areas corresponding to different phases are delimited by bold lines.

In summary, we have studied a tight-binding model on a square lattice ribbon with hopping anisotropy $(t_\uparrow, t_\downarrow, t)$. It is shown that the three different phases may develop: 1) simultaneous occurrence of two edge states with different length scales, 2) simultaneous occurrence of two bulk states with different oscillation lengths; and 3) coexistence of one edge and one bulk state. Simultaneous occurrence of two edge states may appear in three different versions denoted by E_c, E, $E_\pm$. In the first version (E_c), the roots $z_{1,2,3,4}$ are complex causing the eigenstate (2.11) to be complex as well and therefore carrying an electric current. In the rest two versions (E and $E_\pm$), the roots are all real, hence the eigenstate (2.11) is real thus implying no electric current. The detailed study of the current-carrying states (version E_c) will be discussed elsewhere.

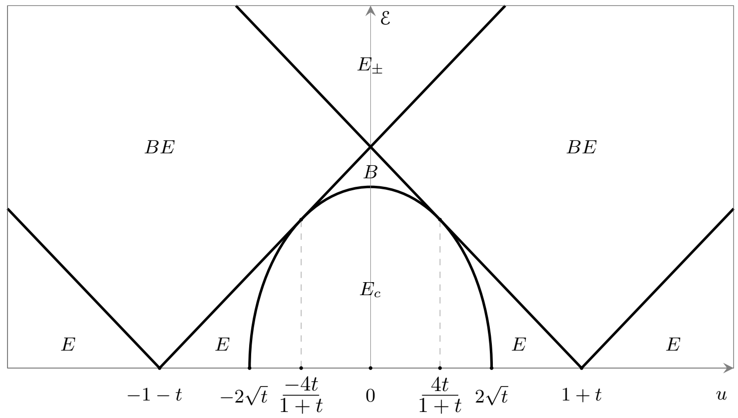

FIGURE 2

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