Flat Energy Bands within Antiphase and Twin Boundaries and at Open Edges in Topological Materials

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A model for two-dimensional electronic, photonic, and mechanical metamaterial systems is presented, which has flat one-dimensional zero-mode energy bands and stable localized states of a topological origin confined within twin boundaries, antiphase boundaries, and at open edges. Topological origins of these flat bands are analyzed for an electronic system as a specific example, using a two-dimensional extension of the Su-Schrieffer-Heeger Hamiltonian with alternating shift of the chains. It is demonstrated that the slow group velocities of the localized flat band states are sensitively controlled by the distance between the boundaries and the propagation can be guided through designed paths of these boundaries. We also discuss how to realize this model in metamaterials.

Flat dispersionless energy bands with infinite effective mass, either in electronic, photonic, or mechanical materials, give unique properties to these materials, and have attracted great attention in the recent past [1–4]. Prominent examples include localized photons in the Lieb photonic lattice [5–7], the Mott phenomena and unconventional superconductivity in twisted bilayer graphenes [8, 9], and the proposal of zero-group-velocity mechanical metamaterials [10]. Another class of materials attracting great attention lately are topological materials, which include topological insulators and semimetals [11–14], phononic materials [15] and metamaterials [10, 16–22]. Since widely different systems could share phenomena of the same topological origin, the tight binding electronic Hamiltonian for the Hal-dane model of graphene [23] has been translated to equations describing topological phenomena in photonic, sonic, and mechanical metamaterials, as well as ultracold fermions [17, 20, 24–26], for example.

In this Letter, we propose a two-dimensional (2D) model system, for which topologically protected flat energy bands arise within the twin boundaries (TB) or the antiphase boundaries (APB), or at the open edges (OE). The flat bands are located in the energy gap between bulk bands, which allows the formation of stable localized states. It is also demonstrated that the group velocity is tunable by the distance between the boundaries and the propagation can be guided through zig-zag paths, unlike other lattices with flat bands. We use an electronic tight-binding Hamiltonian as a specific model, and discuss how the same phenomena could be found in metamaterials.

One of the earliest models of the topological insulators is the 1D Su-Schrieffer-Heeger (SSH) model [21, 27, 28], for which topologically protected zero energy states could be present at the OE or APB. Extension of the SSH model to the 2D space has been studied by simply stacking the 1D SSH chain in the direction perpendicular to the chain [29], which results in dispersive topological edge states. In our study, we extend the 1D SSH model to the 2D space in a different way by shifting every other 1D SSH chain. To be specific [30], a 2D square lattice is altered first by a uniform square-to-rectangle distortion parameterized by $e$, and then by staggered distortions parameterized by $d_x$ and $d_y$, specifically for $A$ atom. Uniform distortions are parameterized by $e$, so that $1 + e$ and $1 - e$ are the distances between neighboring $A$ and $B$ sites in vertical and horizontal directions respectively, before staggered distortions are introduced. The green arrows represent primitive vectors $a_1$ and $a_2$, and the gray ellipses indicate unit cells.

As shown in Fig. 1, a two-atom unit cell is chosen with the unit cell index $n = (n_1, n_2)$ representing the unit cell at $R = n_1 a_1 + n_2 a_2$ with primitive vectors $a_1$ and $a_2$. Two atoms in the unit cell are labeled as $A$ and $B$. The parameters $d_x$ and $d_y$ specifically represent the staggered components of the distortion of $A$ atom. The primitive vectors and unit cells are chosen so that one of the primitive vectors is parallel to the boundary and unit cells are not cut through by the boundaries [29]. By considering one spinless electron state at each site, we obtain the following tight binding Hamiltonian for the...
lattice without APB/TB/OE,
\[ H = -(1 - e + 2d_x)\sigma_+ \otimes I - (1 - e - 2d_x)\sigma_- \otimes S_1 \\
- (1 + e + 2d_y)\sigma_+ \otimes S_2 \\
- (1 + e - 2d_y)\sigma_- \otimes S_1S_2 + H.c, \tag{1} \]
where \( S_j = \sum_n |n\rangle\langle n|, \sigma_+ \) and \( \sigma_- \) are the raising and lowering operators of Pauli matrices, and \( (1, 0)^T \otimes |n\rangle = |A, n\rangle, (0, 1)^T \otimes |n\rangle = |B, n\rangle \) are electron states at corresponding sites. The hopping amplitude for undistorted lattice and the linear coefficient of the hopping amplitude versus the interatomic distance are chosen as 1 and -1, respectively. In various configurations with TB/APB/OE, the coefficients in Eq. (1) become site-dependent, \( t_{nm} \).

The band structure is given by \( H = \sum_{k_1,k_2} [h(k_1,k_2)\sigma_- + h^*(k_1,k_2)\sigma_+] \otimes |k\rangle\langle k|, \tag{3} \)
where \( k = (k_1/2\pi)b_1 + (k_2/2\pi)b_2 \) with \( b_1 \) and \( b_2 \) representing reciprocal lattice vectors, and \( h(k_1,k_2) = -(1 + e + 2d_x)e^{-ik_2} - (1 - e - 2d_y)e^{ik_1+k_2} - (1 - e + 2d_y) \). The band structure is given by \( e_{ik}(k_1,k_2) = (-1)^l[h(k_1,k_2)] \) with \( -\pi < k_1 \leq \pi, -\pi < k_2 \leq \pi \), and the band index \( l = 1, 2 \). For the lattice with a horizontal (vertical) rectangular distortion and \( y \)-directional \( x \)-directional staggered distortions, that is, \( e > 0, d_x = 0, d_y \neq 0 \) \( e < 0, d_x \neq 0, d_y = 0 \), a gap opens between the two bands and the system becomes an insulator for the half-filling. Topology of the system is characterized by the winding number \( \nu \) \([29, 36]\) defined as
\[ \nu(135° \text{ or } 0°) = \frac{1}{2\pi i} \int_{0}^{2\pi} dk_2 \frac{\partial}{\partial k_1} \ln h(k_1,k_2), \tag{4} \]

where \( k_1 = k_1 \) and \( k_2 \) are for boundaries in 135° and 0° directions, respectively. The calculated winding number \( \nu(135°) \) and \( \nu(0°) \) are shown in Table I for four possible equivalent distorted insulating states, which reveals that the winding number depends on the signs of the distortions, and the zero modes would be present for TB/APB/OE separating domains of different winding numbers, as discussed in more detail below.

We present the results obtained by numerical methods for various TB/APB/OE. The distortion patterns are obtained by relaxing atomic-scale model lattice energy expressions with an anharmonic coupling between uniform and staggered distortions, as described in Supplemental Material \([37]\). Because flat energy bands of zero-modes arise from topological origins, the details of TB/APB/OE configurations do not have much effect on the results presented here. Calculations are carried out for systems of 32 × 32 unit cells with periodic boundary conditions and four \( [0,0] \) boundaries in 135° \([0°]\) directions. Only parts of the distorted lattices are shown in Figs. 2 and 3 for clarity, with the labels in each domain representing the signs of \( e, d_x, \) and \( d_y \).

First, we analyze electronic properties of TB. It is well known that only TB along either 45° or 135° direction with respect to the direction of rectangular distortion are stable due to compatibility conditions \([38, 39]\). Figures 2(c) and 2(d) show TB along 135° direction between domains with horizontal and vertical rectangular distortions. The difference between the configurations in Figs. 2(c) and 2(d) is that the staggered distortions, \( d_x \) in the \( e < 0 \) domain and \( d_y \) in the \( e > 0 \) domain, have opposite signs in Fig. 2(c) but the same sign in Fig. 2(d). Therefore, the winding numbers \( \nu(135°) \) for two domains separated by TB are different by one for Fig. 2(c), but identical for Fig. 2(d). By solving the electronic Hamiltonian numerically, we obtain band structure \( e_m(k_2) \) with \( m = 1, \ldots, 64 \), shown in Figs. 2(a) and 2(b). Zero-mode bands are present in the bulk band gap for Fig. 2(a), while absent for Fig. 2(b). The integrated electron density of the zero-mode states are shown on the lattice in Fig. 2(c) in colors, with red and blue colors indicating \( A \) and \( B \) sites, respectively. The results show that these states are localized at TB, on the \( A \) sites for the lower TB and the \( B \) sites for the upper TB. The system has one TB state per TB at each \( k_2 \) point, and satisfies the topologi-
FIG. 2. (color online) (a), (b) Band structures for the lattice with TB shown (c) and (d), respectively. TB zero-mode bands are present in (a), but absent in (b). (c), (d) Lattices with TB in 135° direction. Only parts of 32×32 unit cells with periodic boundary conditions are shown for clarity. The labels in each of the domains represent the signs of $e$, $d_x$ and $d_y$, which show the difference between (c) and (d) in the sign of $d_x$ for the middle domain. Red and blue colors in (c) represent the integrated electron density for the zero-mode band states on A and B sites, respectively.

The results for APB are shown in Fig. 3. Unlike the TB, the APB could be formed in any direction. For 135° (or equivalently 45°) direction APB, Table I shows that the winding number $\nu(135^\circ)$ changes by one whenever the staggered distortion $d_x$ or $d_y$ changes its phase. This implies zero-mode flat bands are always present at 135° or 45° APB, consistent with the numerical results in Figs. 3(a) and 3(d). In contrast, the winding number $\nu$ changes by 2 across 0° [90°] direction APB for domains with horizontal [vertical] rectangular distortions with $e > 0$ [$e < 0$], but does not change for domains with...
vertical [horizontal] rectangular distortions with $e < 0$ [$e > 0$], consistent with the presence or absence of zero-mode flat bands at the APB in Figs. 3(b), 3(c), 3(e), and 3(f). Highly dispersive bands inside the gap for the $0^\circ$ APB with vertical rectangular distortions in Fig. 3(c) are not of topological origin, and the integrated electron density for states with $|\varepsilon_m| < 0.1$ in Fig. 3(f) shows equal presence on $A$ and $B$ sites at each APB, unlike APB states of topological origin. It is also found that the presence of zero mode flat bands localized at the OE along $0^\circ$ and 135$^\circ$ directions follows the topological predictions with the winding number outside the OE always zero.

As mentioned at the beginning, the flat bands found for the system could be useful to create stable or slowly moving localized states. While the 2D Lieb lattice provides bands that are flat in the 2D Brillouin zone, our 2D lattice provides bands that are flat in the 1D subspace of the 2D k-space zone for states localized within TB/APB/OE. Such difference gives a unique possibility to our lattice, that is, the tunability of the band dispersion or the group velocity of the localized states by the distance between TB/APB/OE. As a demonstration, we consider a pair of 135$^\circ$ APB, similar to Fig. 3(d) but with a varying number of bonds $\delta$ along the horizontal direction between APB, for 64 x 64 unit cells, and find that the dispersion of the zero-mode bands increases as $\delta$ decreases. The approximate average group velocity is calculated as $c_g = \varepsilon_{\text{APB}}^{\text{max}}(k_2 = 0) - \varepsilon_{\text{APB}}^{\text{max}}(k_2 = -\pi) / \pi$, where $\varepsilon_{\text{APB}}^{\text{max}}(k_2)$ is the largest among the four zero-mode APB state energies. The result of $c_g$ versus $\delta$ is shown in Fig. 3(g), which reveals rapid increase of $c_g$ as $\delta$ decreases below around 15. This tunability could be useful to design devices with controlled speeds of the propagations for the localized states.

To examine whether the propagation of such localized zero-mode states could change their directions without current loss, a pair of zig-zag APB schematically shown in Fig. 4(a) for 64 x 64 atoms are considered, where three domains with a vertical rectangular distortion have the phase of the staggered distortion $d_{x}$ positive, negative and positive from left to right. The actual distortion pattern near the kinks in the area marked in Fig. 4(a) is shown in Fig. 4(c). Electronic energy spectrum for the whole distorted lattice is found numerically and energy eigenvalue $\varepsilon_m$ versus the index $m$ is displayed in Fig. 4(b), which shows that the zero-mode APB states are well separated from bulk states in energy in spite of kinks. The integrated electron density for these zero-mode states shown in Fig. 4(c) in colors (see the caption for Fig. 2) indicates that these modes are confined at one sublattice for each zig-zag APB and the current would not be lost at the kinks. Such patterned metamaterials, for example, optical crystals, could be used to guide slowly propagating localized states along designed paths.

Although we have used electronic Hamiltonian as a specific example, our model can be applied to other systems, such as photonic or mechanical metamaterials or ultracold fermions. Because chirality symmetry is essential, the metamaterials should have identical on-site energies, or resonances, at all sites, including TB/APB/OE, and the nearest neighbor coupling should have the variations of weakly coupled shifted SSH chains as studied here.

In summary, using a 2D model in the weak AIII/BDI topology class with topology-structure coupling, we have demonstrated the presence of flat zero-mode energy bands in the entire 1D Brillouin zone for states localized within TB/APB/OE. It has been found that the flatnesses of these bands and the slow group velocities for the localized zero-mode states could be controlled by the distance between the boundaries and the slow motion of the localized excitations can be guided through a zig-zag path. We propose our model can be realized in various metamaterials, which would open possibilities for unique device applications.

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LATTICE ENERGY FOR RELAXED STRUCTURAL TEXTURES

Lattice distortion field should satisfy the compatibility conditions, that is, the bonds between atoms should not be broken or overlap with each other. Further, abrupt changes in lattice distortions usually cost a lot of lattice energy, and gradual changes of the lattice distortions would be favored energetically. To take both effects into account at the atomic scale, structural textures are obtained by relaxing an energy expression $E_{\text{lattice}}$ written in terms of the atomic scale modes that represent the lattice distortions. Specifically, the distortion of a square lattice with a monatomic basis can be expressed in terms of five distortion modes, $e_1, e_2, e_3, s_x,$ and $s_y$, shown in Fig. S1, as discussed in detail in Refs. [S1–S4]. The energy expression $E_{\text{lattice}}$, which gives rise to the ground states with $e > 0$, $d_x = 0$, $d_y \neq 0$ (equivalently with $e < 0$, $d_x \neq 0$, $d_y = 0$) illustrated in Fig. ?? is as follow

$$E_{\text{lattice}} = E_s + E_l + E_c,$$

(S1)

$$E_s = \sum_i \left[ \frac{B}{2} (s_x^2 + s_y^2) + \frac{G_1}{4} (s_x^4 + s_y^4) + \frac{G_2}{2} s_x^2 s_y^2 \right]_i,$$

(S2)

$$E_l = \sum_i \left[ \frac{1}{2} A_1 e_1^2 + \frac{1}{2} A_2 e_2^2 + \frac{1}{2} A_3 e_3^2 \right]_i,$$

(S3)

$$E_c = \sum_i \left[ C_3 (s_x^2 - s_y^2) e_3 \right]_i,$$

(S4)

where $E_s$ is the energy for the short-wavelength modes including all symmery-allowed terms up to the fourth order, $E_l$ the energy for the long-wavelength modes in the harmonic order, $E_c$ the coupling between the long- and short-wavelength modes, and $i = [i_x, i_y]$ designates coordinates before distortion.

For uniform phase, the energy minimization of $E_{\text{lattice}}$ leads to $e_1 = e_2 = 0$ and $e_3 = -C_3(s_x^2 - s_y^2)/A_3$, and the minimized total energy per site is

$$\frac{E_{\text{lattice}}^\text{min}}{N^2} = \frac{B}{2} (s_x^2 + s_y^2) + \frac{1}{4} \left( G_1 - \frac{2C_3^2}{A_3} \right) (s_x^4 + s_y^4) + \frac{1}{2} \left( G_2 + \frac{2C_3^2}{A_3} \right) s_x^2 s_y^2.$$

(S5)

With $B < 0$, $G_1 - 2C_3^2/A_3 > 0$, $G_2 + 2C_3^2/A_3 > 0$, and $G_2 + 2C_3^2/A_3 > G_1 - 2C_3^2/A_3$, the global energy minimum occurs for $s_x = \pm s_{\text{min}}, s_y = 0$ and equivalently for $s_x = 0$, $s_y = \pm s_{\text{min}}$, where $s_{\text{min}} = \sqrt{BA_3/(2C_3^2 - G_1A_3)}$. For the results in the main text, the parameter values are chosen as $A_1 = 7$, $A_2 = 4$, $A_3 = 6$, $B = -5$, $C_3 = 20$, $G_1 = 180$, and $G_2 = 100$, which satisfy the conditions specified above and give the minimum energy distortion $s_{\text{min}} = 0.327$ and $e_{\text{min}} = 0.357$, equivalently $e = 0.252$ and $d_x = 0.164$, $d_y = 0$ or $d_x = 0$, $d_y = 0.164$ in Fig. ?? For the inhomogenous configurations with TB and APB, the constraints among $e_1(k)$, $e_2(k)$, $e_3(k)$, $s_x(k)$, and $s_y(k)$ should be considered.

![FIG. S1: Atomic scale distortion modes for a square lattice [S1–S4]. The modes $e_1$, $e_2$ and $e_3$ are long wavelength modes, and the modes $s_x$ and $s_y$ are short wavelength modes.](image-url)
as done in Refs. [S1–S4]. With appropriately chosen initial configurations, the lattice configuration is relaxed using the Euler method applied to $E_{\text{lattice}}$ to obtain the atomic scale profiles of TB, APB, and the zig-zag boundaries in Figs. ??-?? of the main text.

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