Universal edge bands induced by linearly polarized irradiation on phosphorene

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Abstract
Phosphorene (a monolayer of black phosphorus) is a large gap semiconductor with high mobility and has great application potential. Numerical calculations reveal that phosphorene is a topologically trivial material and can only host edge bands on specified edges such as the zigzag edge. A linearly polarized irradiation on the phosphorene lattice results in the dynamic gaps in the quasi-energy spectrum. We found that the irradiation polarized in the zigzag direction induces new edge bands within the dynamic gaps on any type of edge (zigzag, armchair, or other bearded edge). We proposed a new gauge independent quantity, $\delta + g$, to account for the appearance of universal edge bands, where $\delta$ is the detune and $g$ is the light induced valence-conduction band transition element. The number of edge bands in the dynamic gaps is reflected by the winding number of it.

1. Introduction

Periodically driving can turn a normal material into the so-called Floquet topological insulator [1–5]. Light irradiation is an important periodic driving source and its impact on materials draws much attention. Recently, the Floquet topologic phase of condensed matter materials and photonic crystals were observed experimentally [6, 7], and verified the validity of the theoretical prediction and showed the potential application of irradiation for topologic phase engineering. Light irradiation affects the bulk band structure of materials by two mechanisms. First, the electron near the neutral point of gapless materials, such as graphene, emits a photon and re-absorbs it to renormalize the band structure, and so a mini-gap is generated at the neutral point [8–11], which is a second order effect. Secondly, light induces resonant transition between conduction band and valence band states, and results in dynamic gaps in the quasi-energy spectrum at $E = \pm h\omega/2$, where $\hbar$ is the reduced Planck constant and $\omega$ is the angular frequency of light [12–15]. The latter is more attractive because it is a first order process and will be considered in this paper. If the light is circularly polarized, it can change the material’s topological property, which is reflected by the arising of new helical edge bands in the dynamic gaps [14–17]. These photon-exited spectrums can be detected by the Angle-resolved photoemission spectra measurement [7]. Because the illuminated system is not an equilibrium one, the occupation rule of the quasi-energy spectrum is complicated, and the edge band induced by irradiation does not carry exactly one conductance quanta in electronic transport [18–22].

Phosphorene, a monolayer of black phosphorus, has great potential for electronic application because its field-effect transistors have a large on-off current ratio at room temperatures [23–25]. Its energy gap is moderately large and its anisotropy is quite strong. By applying static strain, phosphorene can be tuned into a band-inversion material [26, 27], which could host topological node-line states near the Fermi energy [28]. Vertical electric field can make phosphorene become a Dirac semimetal [29] and induces a topological phase transition in few-layer phosphorene [30]. The linearly polarized laser illumination results in dynamic gaps in the quasi-spectrum of phosphorene, but cannot induce topological phase transition [31]. In this paper, we
investigated the band structure of phosphorene ribbons under linearly polarized irradiation. We found that in the dynamic gaps, there exist edge bands on both zigzag and armchair edges if the polarization is along the zigzag direction, but no edge band appears when the polarization is along the armchair direction. Whether or not edge bands exist in the dynamic gaps is governed by a gauge independent quantity, \( \delta + g \), with \( \delta \) being the detune and \( g \) being the light induced valence-conduction band transition element. For the polarization along other directions, the zigzag component and the armchair component of the polarization vector compete with each other. When the polarization is deviated from the zigzag direction, the \( \mathbf{k} \)-interval of edge band existence shrinks and it vanishes for a critical polarization orientation.

2. Hamiltonian

The phosphorene lattice is composed of puckered-up and puckered-down phosphorus atoms as demonstrated in Figure 1. The in-plane structure of the phosphorene is a deformed honeycomb lattice with the in-plane parameters \( a = 0.8014 \), \( b_x = 1.515 \), and \( b_y = 1.674 \) (in units of Å) \(^{32}\). The \( x \)-axis and \( y \)-axis are set to be parallel to the armchair and zigzag directions. Because there is no difference between the on-site potentials on the puckered-up and puckered-down atoms, the phosphorene lattice can be regarded as a bipartite system consisting of \( A \) and \( B \) sublattices, as shown in the inset. The five types of nonzero hoppings are labeled by \( t_1 \), \( t_2 \), \( t_3 \), \( t_4 \) and \( t_0 \) in the figure, the values of which are 3.665, \(-1.220\), \(-0.205\), \(-0.005\) and \(-0.105\) (in units of eV), respectively \(^{33}\). The tight-binding Hamiltonian reads

\[
H = \sum_{ij} t_{ij} c_i^\dagger c_j,
\]

where the summation runs over all nonzero hoppings. In basis of \( A-B \) sublattices, the \( \mathbf{k} \)-space Hamiltonian is

\[
H_\mathbf{k} = \begin{pmatrix}
 h_0 & \mathbf{h} \\
 \mathbf{h}^* & -h_0
\end{pmatrix},
\]

The elements \( h_0 \) and \( h \) are both of the form

\[
\sum_\alpha t_\alpha e^{i \mathbf{k} \cdot \mathbf{r}_\alpha},
\]

where \( \mathbf{r}_\alpha \) denotes the position vector from an \( A \)-site pointing to nearby \( A \)- or \( B \)-site, and \( t_\alpha \) is the corresponding hopping. The matrix elements are calculated as

\[
h_0 = 4t_0 \cos k_x d_x \cos k_y d_y,
\]

\[
h = e^{ik_\alpha} [t_1 + 2(t_2 e^{-ik_\alpha} + t_3 e^{ik_\alpha}) \cos k_y d_y + t_4 e^{-i2k_\alpha} d_y],
\]

where \( d_x = a + b_x \) and \( d_y = b_y \). Solving the Hamiltonian, we have the conduction band and valence band energies

\[
\epsilon_c = h_0 + |h|, \quad \epsilon_v = h_0 - |h|,
\]

and the corresponding eigen states

\[
|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{-i\theta} \end{pmatrix}, \quad |\phi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix},
\]
where \(|c\rangle\) and \(|\nu\rangle\) are the conduction and valence band states respectively, and \(\phi\) is the complex angle of \(\hbar\). When a polarized light irradiates normally on the phosphorene sheet, the light can be described by a time-dependent vector potential \(A \cos \omega t\), where \(A\) is the amplitude vector and \(t\) is the time. The vector potential can be involved into the Hamiltonian by the Peierls substitution (Form here on, \(h\) and \(e\) in equation expressions are set to be unit to simplify the derivation)

\[ t_n \rightarrow t_n e^{i A \cdot r_n \cos \omega t} \approx t_n (1 + i A \cdot r_n \cos \omega t) \]  

(7)

This leads to the additional time-dependent Hamiltonian

\[ H(t) = A \cdot \nabla \cos \omega t. \]  

(8)

In basis of \(|c\rangle\) and \(|\nu\rangle\), we apply the rotating wave approximation and have the Hamiltonian

\[ H_e = \begin{pmatrix} \epsilon_c & \frac{1}{2} g e^{-i\phi} \\ \frac{1}{2} g e^{i\phi} & \epsilon_\nu \end{pmatrix} \]  

(9)

where \(g\) is the transition element defined by

\[ g = A \cdot \langle c | \nabla \cos \omega t | \nu \rangle. \]  

(10)

One can verify that \(\langle c | \nabla \cos \omega t | \nu \rangle\) is a pure imaginary quantity (see the appendix). Breviate \(\langle c | \nabla \cos \omega t | \nu \rangle\) as \(i\phi\) and we have

\[ g = i A \cdot \nu. \]  

(11)

The time-dependent Shrödinger equation of the Hamiltonian \(H_e\) can be numerically solved in the Floquet space in basis of \(|(c, \nu) e^{i\theta(t)}\rangle\) with \(\theta\) being an integer. The quasi-spectrum can be obtained by averaging the density of states over a period of driving. In this paper, we instead use the method described in [31] to calculate the quasi-spectrum of phosphorene ribbons. The studied armchair and zigzag ribbons lie along \(x\) and \(y\) directions, respectively, according to the axis definition in figure 1.

Figures 2(a)–(d) show the quasi-spectrum for phosphorene ribbons under the irradiation polarized along \(x\)- and \(y\)-directions. In the band gap of the zigzag ribbon, the nearly flat edge bands survive but are disturbed a little by the irradiation, which is not our target in this paper. (The origination of the edge bands of un-irradiated phosphorene ribbons was discussed in [34] and [35], which can be explained by the winding number analysis of \(\hbar\) by choosing proper gauges for the armchair and zigzag edges respectively. The winding number reflects the number of edge bands and was proven to be 0 for armchair ribbons and 1 for zigzag ribbons.) Within the conduction or valence band, the irradiation induces the so-called dynamic gap. Interestingly, one can find that new edge bands appear in the dynamic gaps if the polarization is along \(y\)-direction (the zigzag direction) regardless of the edge type of the ribbons. This means there must be a new gauge invariance to govern the existence of those edge bands, which will be explored in the following.

3. Spectrum and edge bands

To find out the physics within the dynamic gaps, we use the time-dependent unitary transformation

\[ U_t = \begin{pmatrix} e^{-i(\delta - \frac{\phi}{2})t} & 0 \\ 0 & e^{-i(\delta + \frac{\phi}{2})t} \end{pmatrix} \]  

(12)

where \(\delta = (\epsilon_c - \epsilon_\nu) - \omega\) is the detune, to reduce the time-dependent Hamiltonian \(H_e\) into a static one, saying

\[ H_{dc} = U_t H_t U_t^* + i U_t \frac{\partial U_t^*}{\partial t} \right) \]  

(13)

\[ = \frac{1}{2} \begin{pmatrix} \delta & g \\ g^* & -\delta \end{pmatrix}. \]

By means of the unitary matrix

\[ U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \]  

(14)

3 The quasi-spectrum is composed by weighted quasi-energy band dispersions. The dispersion weight is often indicated by the transparency of the dispersion curves [14, 31]. To avoid the obscure of the curves with different transparency and to make the figures more clear, the quasi-energy dispersions with the weight greater than 0.4 are plotted in solid lines, and those with the weight less than that value are invisible in this paper.
we transform the reduced Hamiltonian $H_{rdc}$ into

$$H_{\text{eff}} = U H_{rdc} U^+ = \begin{pmatrix} 0 & \eta^* \\ \eta & 0 \end{pmatrix}$$

with

$$\eta = \delta + g + i A \cdot \mathbf{v}.$$ 

The eigen values of the effective Hamiltonian $H_{\text{eff}}$ are $E_{\pm} = \pm \sqrt{\delta^2 + |g|^2}$. Because $H_{\text{eff}}$ is deduced from the original time-dependent Hamiltonian $H_t$ without approximation, all the information of the irradiated system is encoded in the effective Hamiltonian. Figures 2(e)–(h) show the dispersion of $H_{\text{eff}}$ for the irradiated phosphorene ribbons with zigzag and armchair edges. The features of the quasi-energy bands of $H_t$ can be found in the band structure of $H_{\text{eff}}$: the two dynamic gaps for $H_t$ merge in the spectrum of $H_{\text{eff}}$ and so do the edge bands.

The winding number of the effective Hamiltonian can be used to handle the edge bands of the ribbons. The complex quantity $\eta$ has the real part $\delta$ and the imaginary part $\mathbf{A} \cdot \mathbf{v}$. For a ribbon lying along $x$ direction (armchair ribbon), $k_x$ is a good quantum number. At a given quantum number $k_x$, $\eta$ is a function of parameter $k_y$. When the parameter $k_y$ changes though out the Brillouin zone, the endpoint of the complex vector of $\eta$ on the complex plane moves and evolves as a closed curve. The turn of times of the curve around the origin is called the

Figure 2. (a–d) Quasi-energy band structure of $H_t$, (e–h) band structure of $H_{\text{eff}}$, (i–l) components of $\mathbf{v}$ at resonance as functions of wavevector, and (m–p) winding number pictures of $\eta$ for the wavevectors labeled by the bold dots. Both the armchair and zigzag phosphorene ribbons have 200 transversal atoms. The ribbons are irradiated by linearly polarized light with the frequency $\omega = 4$ eV and with polarization amplitude $A_x = 0.1$ for $x$-polarization and $A_y = 0.1$ for $y$-polarization (the in-plane parameter $a$ is treated as the unit length). The vertical dashed lines indicate the the intervals for $v_y^0$, also the intervals for edge band existence.
winding number. Similarly, if the ribbon lies in \( y \)-direction (zigzag ribbon), \( k_y \) is a good quantum number, and trajectory of the endpoint of \( \eta \) is a closed curve when the parameter \( k_y \) changes through out Brillouin zone. To reflect the number of edge bands, the winding number analysis should use different gauges for different types of edge. We consider the gauge transformation \( U_g \) which transforms the operator \( \nabla_z H_{k z} \) to \( U_g (\nabla_z H_{k z}) \Gamma^g \) and translates the state \( |\mu\rangle (\mu = \xi, \eta) \) to \( U_g |\mu\rangle \). According to equation (10), \( g \) keeps unchanged under the gauge transformation, and so \( \eta \) is a gauge invariant. This means that the existence of edge bands in the dynamic gaps is independent of the edge type.

Firstly we consider the irradiation is polarized in \( x \)-direction (the armchair direction). For this case we have \( \eta = \delta + i \nu_x (A_x \) is set to be a unit which has no influence on the winding number analysis). The trajectory of the endpoint of \( \eta \) for the armchair ribbon at the wavevector denoted by the bold dot in figure 2(e) is shown in figure 2(m). Because \( \nu_x \) is even with respect to \( k_x \) and \( k_y \) (see the appendix), the endpoint moves forth and back in a round trip and the closed trajectory curve is reduced into a single line. The curve contains nothing, the winding number is zero, and so no edge state can be found in the dynamic gap. The trajectory for the ribbon of zigzag type at the given wavevector labeled by the bold dot in figure 2(g) is illustrated as figure 2(o). The trajectory curve for this case is reduced to a line again, the winding number is zero, and no edge state exists in the dynamic gap. For both armchair and zigzag ribbons, the intercept of the trajectory of \( \eta \) on the imaginary axis means the value of \( \nu_x \) at resonance \( \delta = 0 \). Because the trajectory curve modifies when the wavevector \( (k_x, k_y) \) depending on the ribbon orientation) varies, the resonant value of \( \nu_x \) is a function of \( k_x \) (or \( k_y \)) [31]. We define the resonant response quantities

\[
\nu_x^0 = |\nu_x|_{k_x=0}, \quad \nu_y^0 = |\nu_y|_{k_y=0}
\]

(17)

to understand the property of dynamic gap. Figures 2(i) and (k) show the function of \( \nu_x^0 \) versus \( k_x \) for the armchair ribbon and that versus \( k_y \) for the zigzag ribbon, respectively. One can see that consistency between the curve shape and the profile of the dynamic gap in the spectrum.

Secondly, we assume that the irradiation polarization is in \( y \)-direction (the zigzag direction), and we have \( \eta = \delta + i \nu_y (A_y \) is set to be a unit). Figures 2(n) and (p) show the winding number pictures at the wavevectors represented respectively by the bold dots in figures 2(f) and (h). The trajectories of \( \eta \) are up-down symmetric closed curves, because \( \nu_y \) is a odd function of \( k_x \) and \( k_y \) (see the appendix). The origin is inclosed by the trajectory for armchair and zigzag ribbons, and correspondingly, edge states can be found in the band structure at the selected wavevectors. The intercept of the trajectory on the imaginary axis is \( \nu_y^0 \), and a finite \( \nu_y^0 \) means the inclusion of the origin. The vertical dashed lines in the figure indicate the interval for \( \nu_y^0 \), also the interval for edge band existence. Figures 2(j) and (l) show the curves of \( \nu_y^0 \) as function of wavevector \( k_x \) for armchair ribbon and \( k_y \) for zigzag ribbon. The curve for either case hits the axis three times, and correspondingly there are three degenerate points in the spectrum (the degeneracy is not exact because of the lateral confinement effect).

We also check the spectrum of the effective Hamiltonian for phosphorene ribbons with other edges (not shown), such as bearded zigzag and bearded armchair, under linearly polarized illumination, and verify our conclusion: if the polarization is along the zigzag direction, edge bands arise in the dynamic gap, and if along the armchair direction, no edge band turns up.

When the polarization is along neither \( x \)- nor \( y \)-direction, we have \( \eta = \delta + i A_x \nu_x + i A_y \nu_y \). The complex number \( \eta \) can be decomposed to \( \delta + i A_x \nu_x + i A_y \nu_y \). The trajectory of the former for the armchair or zigzag ribbon is just the curve in figure 2(n) or (p) amplified along the imaginary axis by the factor \( A_x \). The distance between the intersect points on the imaginary axis is \( 2 A_x \nu_y^0 \). If we pick the latter part up, it lift the amplified curve vertically by the amount \( A_x \nu_y \), but the intersect point distance \( 2 A_x \nu_y^0 \) is not affected by the lift. Figures 3(e) and (f) show the trajectory of \( \eta \) for armchair and zigzag ribbons at the wavevectors denoted by the bold dots. The shape of the trajectory curve of \( \eta \) is deformed and asymmetric, because the lift amount \( A_x \nu_y \) is not a constant when the wavevector varies. In figure 3(e), the lift amount is large enough so that the origin is exposed outside out the trajectory curve. Therefore, there is no edge state at the selected wavevector. For the case of figure 3(f), the lift amount is not such large, the origin is included by the trajectory, and one can find the edge band states in the spectrum at the corresponding wavevector.

The inclusion of the origin is determined by the competition between \( A_x \nu_y^0 \) and \( A_y \nu_x^0 \). If \( A_y \nu_x^0 > A_x \nu_y^0 \), the origin is inclosed in the trajectory curve and the winding number is 1. We define the ratio \( \chi = \nu_y^0 / \nu_x^0 \) as an intrinsic quantity to characterize the response to the polarization and the ratio \( P = A_y / A_x \) to indicate the polarization orientation, and we have condition for edge state appearing as

\[
\chi > \frac{1}{P}.
\]

(18)

Figures 3(c) and (d) show the curves of \( \chi \) versus the wavevector. For a given polarization orientation, one can find the interval for edge states appearing by cutting the curves of \( \chi \) with the horizontal line \( 1/P \) as shown in the figures. The vertical dashed lines is used to illustrate the interval of the edge bands surviving. Now we consider
the polarization is initialized along \( y \)-direction \( (A_x = 0) \), and then turn on \( x \)-component and increase it. The line of \( 1/P \) moves up, the interval of edge bands will shrink and finally disappear when the horizontal line reaches the maximum of the \( \chi \) curve. If the polarization is more deviated from \( y \)-direction, the horizontal line cannot cross the curve of \( \chi \), and the upper and lower bands depart away from each other completely.

4. Conclusion

Linearly polarized irradiation induces edge bands in phosphorene ribbons on any type of edge in the dynamic gaps if the polarization is along the zigzag direction. The appearing of the universal edge bands is determined by the winding number of \( d + g \). It is gauge independent, and thus is unrelated with the edge type.

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Appendix. Symmetry of \( \nu \)

The winding number of \( \eta \) has tight relation with the symmetry of \( \nu \). According to the amiltonian in equation (2) and the eigen states in equation (6), the quantity \( \langle \nu | \nabla \chi H_0 | \nu \rangle \) is calculated as
We proved that $\phi$ is arg $h$. The expression of $h$ in equation (4) ensures the following relations
\begin{align}
    h(-k_x, k_y) &= h^*, \\
    h(k_x, -k_y) &= h,
\end{align}
and correspondingly, we have
\begin{align}
    \phi(-k_x, k_y) &= \arg h(-k_x, k_y) = -\phi, \\
    \phi(k_x, -k_y) &= \arg h(k_x, -k_y) = \phi \tag{A6}
\end{align}

Now we consider the symmetry of the $x$ component of $v$,
\begin{align}
    v_x(-k_x, k_y) &= -\Im \left[ e^{i\phi} \frac{\partial h^*}{\partial (-k_x)} \right] = \Im \left[ e^{i\phi} \frac{\partial h}{\partial k_x} \right] = v_x, \\
    v_x(k_x, -k_y) &= -\Im \left[ e^{-i\phi} \frac{\partial h}{\partial k_x} \right] = v_x \tag{A7}
\end{align}

We proved that $v_x$ is even about $k_x$ and $k_y$. Turn to the $y$ component, we have
\begin{align}
    v_y(-k_x, k_y) &= -\Im \left[ e^{i\phi} \frac{\partial h^*}{\partial k_y} \right] = -v_y, \\
    v_y(k_x, -k_y) &= -\Im \left[ e^{-i\phi} \frac{\partial h}{\partial k_y} \right] = -v_y \tag{A8}
\end{align}

So we verified that $v_y$ is an odd function of $k_x$ and $k_y$.

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\[\langle \psi | \nabla_x H_k | \nu \rangle = \frac{1}{2} e^{i\phi} \left( \nabla_x h_0 \nabla_x h \left( \frac{1}{2} - e^{-i\phi} \right) \right) \tag{A1}\]
\[= \frac{1}{2} \left( -e^{-i\phi} \nabla_x h + e^{i\phi} \nabla_x h^* \right) \tag{A2}\]
\[= -i \Im \left( e^{-i\phi} \nabla_x h \right) \tag{A3}\]

It is pure imaginary, and we have the expression of $\nu$,
\[\nu = -i \Im \left( e^{-i\phi} \nabla_x h \right) \tag{A4}\]

Its symmetry relies on the properties of $h$ and $\phi = \arg h$. The expression of $h$ in equation (4) ensures the following relations
\[h(-k_x, k_y) = h^*, \]
\[h(k_x, -k_y) = h, \tag{A5}\]

and correspondingly, we have
\[\phi(-k_x, k_y) = \arg h(-k_x, k_y) = -\phi, \]
\[\phi(k_x, -k_y) = \arg h(k_x, -k_y) = \phi \tag{A6}\]

Now we consider the symmetry of the $x$ component of $\nu$,
\[\nu_x(-k_x, k_y) = -\Im \left[ e^{i\phi} \frac{\partial h^*}{\partial (-k_x)} \right] = \Im \left[ e^{i\phi} \frac{\partial h}{\partial k_x} \right] = \nu_x, \]
\[\nu_x(k_x, -k_y) = -\Im \left[ e^{-i\phi} \frac{\partial h}{\partial k_x} \right] = \nu_x \tag{A7}\]

We proved that $\nu_x$ is even about $k_x$ and $k_y$. Turn to the $y$ component, we have
\[\nu_y(-k_x, k_y) = -\Im \left[ e^{i\phi} \frac{\partial h^*}{\partial k_y} \right] = -\nu_y, \]
\[\nu_y(k_x, -k_y) = -\Im \left[ e^{-i\phi} \frac{\partial h}{\partial k_y} \right] = -\nu_y \tag{A8}\]
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