Floquet states of Valley-Polarized Metal with One-way Spin or Charge Conductivity in Zigzag Nanoribbons

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Two dimensional Floquet systems consisted of irradiated valley-polarized metals are investigated. For the corresponding static systems, we consider two graphene models of valley-polarized metal, which have staggered sublattice or uniform intrinsic spin-orbital coupling. For the first or second model, the strongly localized edge states at zigzag edge carry one-way spin polarized or one-way charge current around the intrinsic Fermi level, respectively. In the presence of irradiation with appropriate frequency, first-order dynamical gaps are opened around the intrinsic Fermi level. Weakly localized Floquet edge states with energy within the first-order dynamical gaps appear at the zigzag edge of semi-infinite sheet. In narrow zigzag nanoribbon, the Floquet edge states are gapped out by finite size effect, while the strongly localized edge states remain gapless. Thus, the conductivity of the narrow zigzag nanoribbons are determined by the properties of the strongly localized edge states. Specifically, the narrow zigzag nanoribbons of the first or second model have one-way spin or charge conductivity, respectively. These features are confirmed by the quantum transportation calculations.

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I. INTRODUCTION

Floquet theory describes the quantum states of systems with time-periodically driven Hamiltonian, such as optically irradiated graphene [1, 2] or time-periodically strained graphene [3, 4]. Novel types of topological phases have been predicted to appear in dynamical systems of 2D materials of graphene family [5, 13]. One of the motivation to study Floquet states in 2D materials is to construct topologically protected edge states [14–19] for electronic and spintronic applications. Optically irradiated graphene, which has low energy excitations near to K and K’ Dirac points of the Brillouin zone of honeycomb lattice, has Floquet gaps of all order around energy levels \( \varepsilon = \pm \frac{\hbar \Omega}{2} N \) with \( \Omega \) being the optical frequency and \( N \) being an integer. The first-order gaps (the dynamical gaps that are induced by the first-order electron-photon coupling) are around \( \varepsilon = \pm \frac{\hbar \Omega}{2} \), and the second-order gaps are around \( \varepsilon = 0 \). At the edge of the semi-infinite graphene, the topological edge states appear within the first-order and higher-order gaps. Because the first-order gap is larger than the higher-order gaps, we aim to engineer the Floquet systems with first-order gap around the intrinsic Fermi level(\( \varepsilon = 0 \)).

For graphene models with particle-hole symmetric, the Dirac points of both valleys are at \( \varepsilon = 0 \), so that the first-order gap of the corresponding Floquet systems is always around \( \varepsilon = \pm \frac{\hbar \Omega}{2} \). The naive idea is to move the energy level of one Dirac point to \( \varepsilon = \pm \frac{\hbar \Omega}{2} \), such that the first-order gap is moved to \( \varepsilon = 0 \). In order to keep the system being neutral, the energy level of another Dirac point is moved to \( \varepsilon = \mp \frac{\hbar \Omega}{2} \). If the pair of Dirac points are in opposite valleys, the static system is valley-polarized metal(VPM).

This article considers two graphene models of VPM. For the static systems, zigzag nanoribbons of the two models host strongly localized edge states(SLESs) at the zigzag edge, whose band structures connect the two valleys. The first model of VPM is graphene with staggered sublattice intrinsic spin-orbital coupling(SOC). The staggered sublattice intrinsic SOC is found in graphene with proximity coupling to the transition metal dichalcogenides (TMDCs) [21,22]. The SLESs are recently proposed to be pseudohelical edge states(PHESs) [24]. The PHESs carry one-way spin polarized current around \( \varepsilon = 0 \). The second model of VPM is graphene with uniform intrinsic SOC as well as appropriate staggered sublattice on-site potential and magnetic exchange field. The model is more conveniently realized in silicene-like 2D materials [25], because of the large SOC and tunable staggered sublattice on-site potential. The SLESs carry one-way charge current around \( \varepsilon = 0 \). For both models, the bulk states in the zigzag nanoribbons carry spin or charge current that offset the one-way currents of the SLESs. Thus, the conductivity of the zigzag nanoribbons are regular, i.e., spin conductivity is zero, charge conductivities under forward and backward bias are the same.

In the presence of irradiation with appropriate frequency, Floquet systems based on the two models of VPM have first-order gap around \( \varepsilon = 0 \) in the bulk band structures. The zigzag edge of semi-infinite sheet host Floquet edge states, with energy within the first-order gap. The Floquet edge states are weakly localized at the zigzag edge. In the narrow zigzag nanoribbons, the Floquet edge states are gapped out due to finite size effect. On the other hand, the SLESs are negligibly influ-
enced by the irradiation or the finite size effect. Thus, the SLESs become the dominating conductive states around \( \varepsilon = 0 \), which determine the conductivity of the nanoribbons. As a result, the irradiated zigzag nanoribbons of the first or second model exhibit one-way spin or charge conductivity, respectively.

The article is organized as following: In section II, the tight binding model of the VPM on honeycomb lattice with time-dependent Hamiltonian is given. The calculation methods for the Floquet band structure and conductivity are presented. In section III, the numerical result of the Floquet state consisted of the first model of VPM are presented. In section IV, the numerical result of the Floquet state consisted of the second model of VPM are presented. In section IV, the conclusion is given.

II. MODEL HAMILTONIAN AND CALCULATION METHOD

Tight binding model on honeycomb lattice is a general model that describes graphene as well as silicene and germanene. The effect of optical irradiation is described by time-dependent Peierls phases on the nearest and next-nearest neighbors hoppings. The time-dependent Hamiltonian is given as

\[
H = - \sum_{\langle ij \rangle , s} \gamma_{ij}(t) c_{is}^\dagger c_{js}^\dagger + i \sum_{\langle ij \rangle , s, s'} \lambda^f_{ij}(t) \nu_{ij} [\hat{s}_z]_{ss'} c_{is}^\dagger c_{js}^\dagger + \Delta \sum_{i, s} \xi_i c_{is}^\dagger c_{is} + \lambda_M \sum_{i, s, s'} [\hat{s}_z]_{ss'} c_{is}^\dagger c_{is}^\dagger
\]

where \( \langle ij \rangle \) is index of lattice site, \( s(s') = \pm 1 \) is spin index, \( \gamma_{ij}(t) = \gamma_0 f_{ij}(t) \) is the time dependent nearest neighbor hopping energy with \( \gamma_0 \) being the hopping parameter and \( f_{ij}(t) \) being the time-dependent function, \( c_{is}^\dagger \) is the creation(annihilation) operator of electron at the \( i-th \) lattice site with spin \( s \), \( \hat{s}_z \) is the creation(annihilation) operator of electron at the \( i-th \) lattice site with spin \( s \), \( s_z \) is the spin-z Pauli matrix, and \( \nu_{ij} = \pm 1 \) for clockwise or counterclockwise next nearest neighbor hopping. The summation with indices \( \langle ij \rangle \) \( \langle \langle ij \rangle \rangle \) is the nearest neighbor(largest nearest neighbor) lattice site. The value of \( \gamma_0 \) is 2.8, 1.6, 1.3 eV for graphene, silicene, germanene, respectively. \( \lambda^f_{ij}(t) \) is equal to \( \lambda^f_{ij} f_{ij}(t) \) and \( \lambda^B_{ij} f_{ij}(t) \) for A and B sublattice, respectively, which also include the time-dependent function \( f_{ij}(t) \). \( \Delta \) is the strength of the staggered sublattice on-site potential, and \( \xi_i = \pm 1 \) for A and B sublattice. In graphene, \( \Delta \) could be induced by the h-BN or SiC substrate; in silicene and germanene, \( \Delta \) is induced by the vertical static electric field \( E_z \). Because of the buckler structure of silicene and germanene, the A and B sublattice planes are separated by \( 2l \), so that \( \Delta = E_z l \). The exchange field \( \lambda_M \) is induced by proximity with ferromagnetic insulator. \( \Delta \) and \( \lambda_M \) are not time-dependent. For the corresponding static systems, the first model of VPM has parameters: \( \lambda_M^A = -\lambda_M^B = \lambda_I \), \( \Delta = 0 \) and \( \lambda_M = 0 \); the second model of VPM has parameter: \( \lambda_M^A = \lambda_M^B = \lambda_I \) and \( \Delta = \lambda_M = 3\sqrt{3} \lambda_I \). In addition to the graphene-like 2D materials, the two models could be experimentally realized in cold atomic systems.\[23–31\].

In the presence of the normally incident optical field with the in-plane electric field being \( \mathbf{E} = \hat{x} E_x \sin(\Omega t) + \hat{y} E_y \sin(\Omega t - \varphi) \), the time-dependent function of the nearest neighbor hopping terms are given as

\[
f_{ij}(t) = \exp\left\{ \frac{2\pi}{\Phi_0} \int_{R_1} A(r, t) \cdot \mathbf{r} \right\}
\]

\[
= \exp\left\{ \frac{2e}{\hbar \Omega} [E_x \hat{x} \cdot \mathbf{r}_{ij} \cos(\Omega t) + E_y \hat{y} \cdot \mathbf{r}_{ij} \cos(\Omega t - \varphi)] \right\}
\]

where \( \Phi_0 \) is the magnetic flux quantum, \( r_{ij} = r_j - r_i \) with \( r_i \) being the location of the \( i-th \) lattice site. The time-dependent function of the intrinsic SOC \( f_{ij}(t) \) has the same form. In this article, we consider only the circular polarized optical field with \( E_x = E_y = 0 \) and \( \varphi = \pi/2 \). According to the Floquet theory, the Floquet state is time periodic function being written as \( |\Psi_\alpha(t)\rangle = e^{-i\varepsilon_\alpha t/\hbar} \sum_{m=-\infty}^{+\infty} |u_m^{\alpha}\rangle e^{im\Omega t} \), with \( \varepsilon_\alpha \) being the quasi-energy level of the \( \alpha \)-th eigenstate and \( |u_m^{\alpha}\rangle \) being the corresponding eigenstate in the \( m \)-th Floquet replica. The Floquet states and the corresponding quasi-energy level are the solution of the equation

\[
H_F |\Psi_\alpha(t)\rangle = \varepsilon_\alpha |\Psi_\alpha(t)\rangle
\]

where \( H_F = H - i\hbar \frac{\partial}{\partial t} \) is the Floquet Hamiltonian. The time-dependent factor in the Hamiltonain can be expanded by the set of time periodic function \( e^{im\Omega t} \) as

\[
f_{ij}(t) = \sum_{m=-\infty}^{+\infty} f_{ij}^m e^{im\Omega t} e^{-i\varphi
\]

\[
= \sum_{m=-\infty}^{+\infty} f_{ij}^m \left( \frac{2e E_x}{\hbar \Omega} \hat{x} \cdot \mathbf{r}_{ij} \right) J_{m-m'}(\frac{2e E_y}{\hbar \Omega} \hat{y} \cdot \mathbf{r}_{ij}) e^{im'\varphi}
\]

where \( J_m(x) \) is the m-th order first type Bessel function of argument \( x \). Similar expansion is applied to \( f_{ij}(t) \). In the direct product space(Sambe space), \( \mathbf{R} \otimes \mathbf{T} \), with \( \mathbf{R} \) being the Hilbert space and \( \mathbf{T} \) being the space of time periodic function, the set of functions \( \{ |u_m^{\alpha}\rangle, m \in \mathbb{N} \} \) form the time-independent basis functions of the Floquet states. In this space, the Floquet Hamiltonian can be expressed as time-independent block matrix, \( \mathcal{H}^{(m,m)} \), with \( m_1 \) and \( m_2 \) being the indices of replicas. The diagonal blocks \( \mathcal{H}^{(m,m)} \) include three parts: the nearest and next nearest neighbor hopping terms, whose hopping coefficients are renormalized by the factor \( f_{ij}^0 \) and \( f_{ij}^0 \), respectively; the staggered sublattice on-site potential and magnetic exchange field; and the diagonal matrix \( m \hbar \Omega \mathbf{I} \). The non-diagonal block includes the nearest and next nearest neighbor
hopping terms, whose hopping coefficients are renormalized by the factor $i_{m_2-m_1} f_{m_2-m_1} e^{-i(m_2-m_1)\varphi}$ and $i_{m_2-m_1} f_{m_2-m_1} e^{-i(m_2-m_1)\varphi}$, respectively. The quasi-energy band structures of bulk or nanoribbon of the model can be obtained by diagonalization of the Floquet Hamiltonian with appropriate Bloch periodic boundary condition. For the eigenstate of the $\alpha$-th quasi-energy, the weight of the static component (the $m = 0$ replica) is given as $\langle u_0^i | u_0^f \rangle$. In the numerical calculation, the Floquet index $m$ is truncated at a maximum value with $m \in [-m_{\text{max}}, m_{\text{max}}]$. In general, calculation with larger $m_{\text{max}}$ gives more accurate result. If the investigation focuses on the first-order gap of the quasi-energy dispersion in the $m = 0$ replica, $m_{\text{max}} = 2$ gives sufficient accurate result, because all single-photon transitions to the dynamical gap are considered. Similarly, if the investigation focuses on the $P$-th order gap, $m_{\text{max}} = 2P$ is required to has sufficient accuracy.

Density of states of semi-infinite sheet with zigzag edge are calculated to visualize dispersion of SLESs and Floquet edge states. Similar to the Floquet Hamiltonian, the Floquet Green’s function can be expressed as time-independent block matrix in the Sambe space, $G^{(m_1,m_2)}$. Local density of state on the $i$-th lattice site is $-\frac{1}{\pi} \text{Im} \langle G^{(0,0)}_{ii} \rangle$. The Floquet Green’s function of the primitive cells at the left or right zigzag edge can be obtained by applying recursive method \[32\ \text{to} \] the Floquet Hamiltonian. Because the edge states are not completely localized at the first primitive cell at the zigzag edge, backward recursive process is performed to calculate the Floquet Green’s function of the primitive cells near to the zigzag edge. Numerical result show that the SLESs are strongly localized at the first primitive cell, while the Floquet edge states are weakly localized. In our calculation, the density of states for each zigzag edge are the summation of the local density of states of the fifty primitive cells near to the corresponding zigzag edge, given as

$$\rho_{\text{left(right)}}(\varepsilon, k_y) = -\frac{1}{\pi} \sum_{\varepsilon \in \text{left(right)}} \text{Im} \langle G^{(0,0)}_{ii} \rangle(\varepsilon, k_y)$$

In reality, the transportation is measured for a zigzag nanoribbon with finite length that is connected to two leads. The structure of the transportation simulation is shown in Fig. 1(a). In our calculation, we construct the scattering region as the zigzag nanoribbon on the x-y plane with width being 2.13 nm and longitudinal length(along y axis) being 73.79 nm. The optical irradiation is restricted in the middle part of the scattering region. The amplitude of the optical field, $E_0$, is assumed to be uniform along x axis, and Gaussian function along y axis as shown in Fig. 1(b). The leads are not irradiated by the optical field, so that both leads are static systems, i.e. VPM. At the buffering unit cells(three unit cells in our calculation) between the leads and the scattering region, $E_0$ is slowly turn on from zero to the small value at the tails of the Gaussian function.

The Floquet Green’s function of the zigzag nanoribbon in the scattering region is calculated by the recursive algorithm \[32\ \text{to} \] \[34\] . For static systems, the transmission coefficient at energy level $\varepsilon$ from lead $L$ to lead $R$ is determined by the Landauer-Buttiker formula, $T_{LR}(\varepsilon) = T \langle \Gamma_L G_{LR}^\dagger(\varepsilon) \Gamma_R \rangle$, with $\Gamma_L(R)$ being the line width matrix of the $L(R)$ lead and $G_{LR}$ being the Green’s function between the lattice sites at the $L$ and $R$ leads. For the Floquet systems, the transmission accompanied by the photon process(absorption or emission) has coefficient $T_{LR}^m(\varepsilon) = T \langle \Gamma_L G_{LR}^\dagger(\varepsilon) \Gamma_R \rangle$, with $\langle \Gamma_L G_{LR}^\dagger(\varepsilon) \Gamma_R \rangle$. The additional superscript $m$ is the index of the Floquet replicas, and $G_{LR}^{(0,m)}$ is the $m$-th row 0-th column block of the Floquet Green’s function. The conductance with Fermi level being $\varepsilon$ under infinitesimal bias from lead $L$ to $R$ is the summation of transmission with all photon processes, $G(\varepsilon) = (2e^2/\hbar) \sum_m T_{LR}^m(\varepsilon)$. With moderate optical intensity, the amplitude of $T_{LR}^m$ decay fast as $|m|$ increase. The transmission of the $m = 0$ replica, $T^0_{LR}$, contribute the major part of the conductance.

### III. Graphene with Staggered Sublattice Intrinsic SOC

The first model of VPM is given by the Hamiltonian $H$ with parameters $\lambda_A = -\lambda_B = \lambda_I$, $\Delta = 0$ and $\lambda_M = 0$. In the reality heterostructure of graphene on TMDCs, the model should include staggered sublattice on-site potential and Rashba SOC in addition. The heterostructure is insulator instead of VPM. Engineering of the heterostructure, such as doping or additional proximity to another substrate, could offset the staggered sublattice on-site potential and Rashba SOC. We focus on the conceptual VPM model without Rashba SOC and with zero or small staggered sublattice on-site potential.
A. Floquet states of bulk

The appropriate optical frequency depend on the model parameters as well as the optical parameters. If $\lambda_I$ is much smaller than $\gamma_0$, the low energy excitations near to K and K’ points of the Brillouin zone can be described by the Dirac Fermion model with Hamiltonian being

$$H = \hbar v_F (\tau \sigma_x k_x + \sigma_y k_y) + \frac{3\sqrt{3}}{2} (\lambda_I^A (\sigma_z + \sigma_0) + \lambda_I^B (\sigma_z - \sigma_0)) \tau_s$$

where $\tau = \pm 1$ stand for K and K’ valleys. Because $\lambda_I^A = -\lambda_I^B = \lambda_I$, the intrinsic SOC terms become a constant potential $3\sqrt{3}\lambda_I \tau_s$. The model has particle-hole-valley symmetric, i.e. the static band structure is symmetric under the simultaneous operation of particle-hole and K-K’ valley exchanges. For the static systems, the energy levels of the Dirac points are $3\sqrt{3}\lambda_I \tau_s$; all four Dirac Fermion models are gapless. The intrinsic Fermi level cut through all Dirac cones at finite energy, so that the model is VPM. Although the particle-hole symmetric is broken, the band structure of each Dirac cone is symmetric about the energy level $3\sqrt{3}\lambda_I \tau_s$. In the Floquet solution with $E_0 = 0$, the band structures of the $m$ replicas are obtained by adding $m\hbar\Omega$ to the static band structures. The crossings between the band structures of all replicas are at energy $\varepsilon = 3\sqrt{3}\lambda_I \tau_s + \frac{1}{2} m\hbar\Omega$. Therefore, the appropriate optical frequency would be $\hbar\Omega = 3\sqrt{3}\lambda_I \times 2$. If $\lambda_I$ is sizable comparing to $f_{\gamma_0}$, the quantum states at $\varepsilon = 0$ cannot be considered as low energy excitation. The static band structures deviate from the linear dispersion of the Dirac cone, such that the band structures are no longer symmetric about the energy level $3\sqrt{3}\lambda_I \tau_s$. Thus, in the Floquet solution with $E_0 = 0$, the crossing between the band structures of all replicas are no longer aligned at energy $\varepsilon = 3\sqrt{3}\lambda_I \tau_s + \frac{1}{2} m\hbar\Omega$. The optical frequency need to be tuned around $\hbar\Omega = 3\sqrt{3}\lambda_I \times 2$, so that the crossings between the bands of $m = 0$ and $m = \pm 1$ replicas align at $\varepsilon = 0$. With $E_0 \neq 0$, the first-order gaps of the quasi-energy band structures are around $\varepsilon = 0$. However, the energy ranges of the first-order gaps in the two valleys are different from each other, so that the global first-order gap is smaller than the first-order gap in each valley. Because the irradiation changes the hopping parameters in the diagonal blocks of the Floquet Hamiltonian by the factors $f_{(i,j)}^\alpha$ and $f_{(i,j)}^\beta$, the energy level of the Dirac points become dependent on $E_0$. As a result, for a given $E_0$, the frequency need to be further tuned to maximized the global first-order gap.

The quasi-energy band structure of spin up electron in the bulk with parameters $\lambda_I = 0.06\gamma_0$ and $E_0 = 0.3V/nm$ is plotted in Fig. 2(a). The band structure of the spin down electron is obtained by mirroring the band structure of the spin up electron about the M point. The optical frequency is tuned to $\hbar\Omega = 3\sqrt{3}\lambda_I \times 1.95$, so that the first-order gaps in K and K’ valleys are in the same energy range. Around energy $\varepsilon = 0$, multiple side bands with small weight in the $m = 0$ replica ($|u_0^\alpha| \ll 1$) are gapless. As a result, the Floquet systems are not insulator. Thus, the topological property is not well defined for this Floquet system. In the additional presence of the staggered sublattice on-site potential, the local static gap of $2\Delta$ at the two Dirac points are opened. Assuming $\Delta = -0.15\gamma_0$, the quasi-energy band structure is plotted in Fig. 2(b). The first-order gaps in the two valleys are both around $\varepsilon = 0$. The gap size at K(K’) valley decreases(increases).

B. Semi-infinite zigzag edge

For a semi-infinite zigzag edge of the irradiated VPM, two types of edge states appear: the SLESs and Floquet edge states. The Floquet edge states only appear in the Floquet systems, with energy within the dynamical Floquet gaps. The SLESs appear in both of the static and Floquet systems. With appropriate model parameters,
the SLESs are negligibly impacted by the irradiation. For the static system of pristine graphene with $\lambda_I = 0$, the bands of the SLESs are the zero-energy flat bands of zigzag edge, which connect the two valleys. The SLESs are strongly localized at the last atom of one zigzag edge and weakly distributed among the other atoms in the same sublattice. With $\lambda_I \neq 0$, the bands of the SLESs become nearly linear dispersive with nonzero slope. For the graphene with staggered sublattice intrinsic SOC, the SLESs are PHESs. The PHESs with the same spin at the left and right zigzag edge travel along the same direction. By contrast, in the quantum spin Hall (QSH) model with uniform intrinsic SOC [39], the SLESs (referred to as helical edge states) with the same spin at the left and right zigzag edge travel along the opposite directions. Because the staggered sublattice intrinsic SOC does not induce band inversion, the PHESs only appear in the zigzag edge, but do not appear in the armchair edge. The bulk band structures along the K-M-K’ line in Brillouin zone (Fig. 2) imply the band edge of bulk states in zigzag semi-infinite sheet or zigzag nanoribbon. One can plot the bands of the PHESs in the bulk band structure (the thick blue lines in Fig. 2), and then estimated the Floquet coupling strength between the bulk states and the PHESs. If the difference between the energy levels of the PHESs and the bulk states is more than $\hbar \Omega$, the PHESs and the bulk states are negligibly coupled by higher order photon transition. The PHESs that satisfy this condition are in the sections of the bands with solid blue lines in Fig. 2. These sections of the bands would remain gapless in the Floquet systems. In contrast, the sections of the bands with dash blue lines would be split by multiple Floquet gaps. For the model with $\Delta = 0$ in Fig. 2(a), the bands of the PHESs around $\varepsilon = 0$ would remain gapless, so that the PHESs are the dominating conductive states. In contrast, for the model with $\Delta = 0.15 \gamma_0$ in Fig. 2(b), the bands of the PHESs around $\varepsilon = 0$ would be split, so that the PHESs are not the dominating conductive states. Thus, small or vanishing staggered sublattice on-site potential is preferred. In the rest of this section, $\Delta = 0$ is assumed.

For the model with $\lambda_I = 0.02 \gamma_0$, $\hbar \Omega = 3 \sqrt[3]{3} \lambda_I \times 1.99$ and $E_0 = 0.1V/nm$, the density of states of the spin up (down) electron at the left and right zigzag edge are plotted in Fig. 3(a) and (b), respectively; those of spin down states are plotted in (c) and (d), respectively. The model parameters are $\lambda^I_L = -\lambda^I_R = \lambda_I = 0.02 \gamma_0$ and $\Delta = \lambda_M = 0$. The optical parameters are $\hbar \Omega = 3 \sqrt[3]{3} \lambda_I \times 1.99$ and $E_0 = 0.1V/nm$. The color scale is normalized to one.

The first-order gaps of the bulk states around $\varepsilon = 0$ are about 0.1 eV. Within the first-order gap, the Floquet helical edge states (FHESs) appear. For the same zigzag edge and the same spin, the FHESs in K and K’ valleys travel along the same direction. The FHESs at the same zigzag edge with different spin travel along the opposite directions. Thus, the FHESs at the two zigzag edges carry spin currents along the opposite directions. The side bands have small density of state around $\varepsilon = 0$, which also contribute to the conductivity along the zigzag edge.

C. spin polarized transport of zigzag nanoribbon

In the narrow zigzag nanoribbons, the appropriate optical frequency depends on the width of the nanoribbons. The band structures of the bulk states and FHESs significantly deviate from those in zigzag edge of semi-infinite sheet (in Fig. 3) due to finite size effect. The finite size

FIG. 3: Density of states for zigzag edge of semi-infinite sheet. $\rho_{\text{left}}(\varepsilon, k_y)$ and $\rho_{\text{right}}(\varepsilon, k_y)$ of spin up states are plotted in (a) and (b), respectively; those of spin down states are plotted in (c) and (d), respectively. The model parameters are $\lambda^I_L = -\lambda^I_R = \lambda_I = 0.02 \gamma_0$ and $\Delta = \lambda_M = 0$. The optical parameters are $\hbar \Omega = 3 \sqrt[3]{3} \lambda_I \times 1.99$ and $E_0 = 0.1V/nm$. The color scale is normalized to one.
The length of the zigzag nanoribbon is finite, and the irradiated region is restricted, as shown in Fig. 4(c). The spin conductivity that is defined as the difference between the conductivities of spin up and down electrons, \(P_G = G_{+1} - G_{-1}\), is plotted in Fig. 4(d). With the backward bias, \(G_{+1}\) and \(G_{-1}\) in Fig. 4(c) exchange, so that the spin conductivity in Fig. 4(d) flips sign. Within the first-order gap, \(P_G\) is peaked near \(2(2e^2/h)\). Thus, forward or backward infinitesimal bias with the Fermi level around \(\varepsilon = 0\) excites spin up or down polarized conductivity, respectively. The spin conductivity at \(\varepsilon = 0\) is not exactly quantized because the side bands contribute small conductivity as well. In the absence of the optical irradiation, both \(G_{+1}\) and \(G_{-1}\) are exactly \(2(2e^2/h)\) at \(\varepsilon = 0\), and the spin conductivity is zero. Therefore, the one-way spin conductivity is controlled by the presence of the optical irradiation.

The optical parameters for experimental implementation of the Floquet system is discussed here. For bulk or semi-infinite sheet, we assume that the graphene is irradiated by normally incident Gaussian beam. If the width of the beam waist is larger than the wavelength, the optical field in the middle of the Gaussian beam could be approximated as plane wave. We denote \(w_0 = w_1\lambda\) as the width of the beam waist with \(\lambda = 2\pi c/\Omega\) being the wavelength and \(w_1 \geq 1\). The power of the Gaussian beam is \(P_0 = \frac{\pi w_0^2}{2}\) with \(\omega_0 = \sqrt{\mu/\varepsilon}\) being the independent of the background media. The first-order gap can be estimated by first order perturbation method as \(\eta h\Omega = \frac{c c/\mu c/\varepsilon}{2}\) with \(\eta < 0.5\) and \(v_F \approx c/330\). Thus, the power of the Gaussian beam is given as

\[
P_0 = \frac{\pi c^2 h^2 \Omega^2 \varepsilon^2 \eta^2}{Z_0 c^2 v_F^2} \approx (30h\Omega w_1 \eta)^2 |W|
\]  

For the model with parameters in Fig. 3 and 4, assuming \(w_1 = 1\) and \(\eta = 0.2\), we have \(P_0 \approx 12\) W. For the system in Fig. 4, the optical field pattern have subwavelength size. Plasmonic devices, such as metallic tip or plasmon cavity[41], could focus the Gaussian beam into subwavelength field pattern. The local electric field is enhanced by a factor, \(F\). Thus, the required power of the laser beam is reduce by \(\sqrt{F}\) times.

IV. GRAPHENE WITH UNIFORM INTRINSIC SOC

The second model of VPM is given by the Hamiltonian with parameters \(\lambda^a = \lambda^b = \lambda_t\) and \(\Delta = \lambda_M = 3\sqrt{3}\lambda_t\). This model is more conveniently realized in 2D staggered semiconductors silicene, germanene, stanene, and plumbene[40].

A. Floquet states of bulk

The appropriate optical frequency depend on the model parameters, but does not depend on the optical
parameters. The low energy excitation near to K and K' points of the Brillouin zone can be described by the Dirac Fermion model, whose Hamiltonian is

\[ H = \hbar v_F (\tau \sigma_x k_x + \sigma_y k_y) \]
\[ + 3\sqrt{3} \lambda_M \sigma_x \tau S + \Delta \sigma_z + \lambda_M \sigma_0 S \]

The model has particle-hole-valley-spin symmetric, i.e. the static band structure is symmetric under the simultaneous operation of particle-hole, K-K' valley and spin up-down exchanges. For the static systems, the energy levels of the Dirac points are \( \lambda_M s \). Two Dirac Fermion models (spin up in K' valley, and spin down in K valley) are gapless; the other two Dirac Fermion models have gap as large as \( 4\lambda_M \). The intrinsic Fermi level cut through the two gapless Dirac cones, which have opposite spin and are in opposite valley. Thus, the VPM exhibit feature of spin-valley locking. With sizable intrinsic SOC, the band structures at \( \varepsilon = 0 \) deviate from the linear dispersion of the Dirac cones. Meanwhile, the band structure of spin-\( s \) electron is symmetric about the energy level \( \lambda_M s \) through out the whole Brillouin zone. As a result, the appropriate optical frequency is exactly \( \hbar \Omega = \lambda_M \times 2 \). In the presence of the irradiation with this frequency, the first-order gaps as well as all higher order gaps of the Floquet quasi-energy band structures are around \( \varepsilon = 0 \). The Floquet systems are insulator. The quasi-energy band structures of the Floquet system with model parameters \( \lambda_M = 0.06 \gamma_0 \) and optical parameters \( E_0 = 0.9V / nm \) and \( \hbar \Omega = 2\lambda_M \) are plotted in Fig. 5.

Because the Floquet systems are insulators, the topological property can be well defined. One can define the Chern number \( C \) of the Floquet systems as

\[ C = \frac{1}{2\pi} \sum_{\alpha \in \text{occupied}} \int_{BZ} 2dk \mathcal{B}_\alpha \]

where \( \mathcal{B}_\alpha \) is the Berry curvature of the \( \alpha \)-th quasi-energy band. The integral cover the whole Brillouin zone. For the Floquet systems, \( \mathcal{B}_\alpha \) is defined as

\[ \mathcal{B}_\alpha(k) = \sum_{\alpha' \neq \alpha} \frac{2Im(\langle \Psi_\alpha(k,t) | v_x | \Psi_{\alpha'}(k,t) \rangle \langle \Psi_{\alpha'}(k,t) | v_y | \Psi_\alpha(k,t) \rangle)}{(\varepsilon_\alpha - \varepsilon_{\alpha'})^2} \]

where \( v_x(y) \) is the velocity operator. The Berry curvature are evaluated at any fixed time. In principle, the wave functions include all Floquet replicas. For numerical calculation, the truncation of the Floquet replicas should satisfies the condition: \( m_{\text{max}} > \text{floor}(6\gamma_0/(\hbar \Omega)) \) with \( \text{floor}[x] \) being the largest integer that is smaller than \( x \). This condition ensures that all dynamical gaps in the whole quasi-energy band are considered. For spin \( s \), the lowest \( 2m_{\text{max}} + 1 - s \) quasi-energy bands are the occupied bands. Within these bands, the lowest \( \text{floor}(6\gamma_0/(\hbar \Omega)) \) bands omit some dynamical gaps due to the truncation. As a result, the summation in Eq. (10) and (11) should include only the \( 2m_{\text{max}} + 1 - s - \text{floor}(6\gamma_0/(\hbar \Omega)) \) bands below the intrinsic Fermi level. Once these conditions are satisfied, the Chern number is independent of the truncation. The numerical results show that the Chern number for each spin is zero, so that the Floquet insulators are topologically trivial.

### B. Semi-infinite zigzag edge

For a semi-infinite zigzag edge of the irradiated VPM, the SLESs appear in both of the static and Floquet systems. Similar to the analysis in Section IIIB and Fig. 2 the bands of the SLESs are plotted in the bulk band structure in Fig. 5 as thick blue lines. For each spin, only one of the two SLESs has band structure that crosses the energy \( \varepsilon = 0 \). For the model parameters in Fig. 5 the bands of SLESs around \( \varepsilon = 0 \) would remain gapless in the Floquet systems. This feature is valid for the realistic systems with smaller strength of the intrinsic SOC.
FIG. 6: Density of states for zigzag edge of semi-infinite sheet. \( \rho_{\text{left}}(\varepsilon, k_y) \) and \( \rho_{\text{right}}(\varepsilon, k_y) \) of spin up states are plotted in (a) and (b), respectively; those of spin down states are plotted in (c) and (d), respectively. The model parameters are \( \lambda_I = \lambda_B = \lambda_I = 0.02 \). The optical parameters are \( \hbar \Omega = \lambda_M \times 2 \) and \( E_0 = 0.1V/nm \). The color scale is normalized to one.

For the model with \( \lambda_I = 0.02 \gamma_0 \), \( \hbar \Omega = \lambda_M \times 2 \) and \( E_0 = 0.1V/nm \), the density of states of the spin up(down) electron at the left and right zigzag edge are plotted in Fig. (a) and (b), respectively. Around \( \varepsilon = 0 \), the SLESs of the two spin components travel along the same direction, so that the SLESs carried one-way charge current; the two SLESs of spin are localized at zigzag edges of opposite sides(opposite sublattice polarization). The Floquet edge states with bands within the first-order gap around \( \varepsilon = 0 \) are denoted as Floquet chiral edge states(FCESs). Being different from the FHEs in the previous model, the FCESs carry charge currents at the zigzag edge. The charge currents at the zigzag edges of opposite sides are opposite to each other.

C. One-way Charge Transport of Zigzag Nanoribbon

In the narrow zigzag nanoribbons, the appropriate optical frequency(\( h\Omega = \lambda_M \times 2 \)) is not changed by the finite size effect, because the static band structure of spin-s is symmetric to the energy level \( \lambda_M s \). For the zigzag nanoribbon with width being 2.13 nm, \( \lambda_I = 0.02 \gamma_0 \), \( E_0 = 0.1V/nm \) and \( h\Omega = \lambda_M \times 2 \), the quasi-energy band structures of spin up and down electron are plotted in Fig. (a) and (b), respectively. The dominating conductive state around \( \varepsilon = 0 \) is the SLESs that carry one-way charge current. As a result, with the Fermi level around \( \varepsilon = 0 \), the charge conductivity under forward or backward bias is expected to be zero or \( 2 \times 2e^2/\hbar \), respectively. The large band gaps of the spin up(down) band structures around the energy \( \pm h\Omega \) are not due to the optical irradiation, but due to the finite size effect. The optical irradiation induces the Floquet side bands within these gaps.

The conductivity of the zigzag nanoribbon with finite length(300 unit cells along the longitudinal direction) and restricted irradiated region in the scattering region is calculated. The charge and spin conductivities under infinitesimal bias versus the Fermi level are plotted in Fig. (c) and (d), respectively. The conductivities under forward and backward bias are plotted as solid(blue) and...
dash(red) lines, respectively. At \( \varepsilon = 0 \), the only conductive states are the SLESs that travel along backward direction, so that the conductivity under forward bias should be zero. However, the calculated conductivity is not exactly zero at \( \varepsilon = 0 \). The small length of the irradiated region allow significant tunneling between the leads. For the scattering region with 900 unit cell, the charge conductivity is reduced to \( 10^{-6} \times 2e^2/h \). Under backward bias, the SLESs contribute quantized conductivity around \( \varepsilon = 0 \). The nonzero spin conductivity appear at energy away from \( \varepsilon = 0 \). The plateaus of quantized spin conductivity around \( \pm \frac{\Delta \varepsilon}{2h} \) are due to the finite size effect, but not due to the optical irradiation. The dips in these plateaus are due to the side bands that are induced by the irradiation. The irradiation induces other dips and peaks in the charge and spin conductivity, including the two peaks of spin conductivity around \( \varepsilon = 0 \) near to the band edge of the first-order gap. All of these dips and peaks are due to the presence of the Floquet side bands with small weight on the \( m = 0 \) replica.

V. CONCLUSION

In conclusion, the Floquet systems of optically irradiated VPMs consisted of 2D graphene-like materials are investigated. Two graphene models of VPM are considered. For the corresponding static systems, the SLESs of the first(second) model carry one-way spin polarized(one-way charge) current. By choosing the appropriate optical frequency and strength, the Floquet systems have first-order dynamical gap around the intrinsic Fermi level, which gap out the conductive bulk states in bulk, semi-infinite sheet or nanoribbon. At the zigzag edge of semi-infinite sheet, the conductive states are the SLESs, Floquet edge states and side bands. In narrow zigzag nanoribbons, the conductive states are SLESs and side bands. The conductivities of the side bands are negligible, so that the conductivities of the narrow zigzag nanoribbons are basically determined by the properties of the SLESs. As a result, the one-way spin or charge conductivities are optically induced.

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