

Off-resonant light-induced topological phase transition and thermoelectric transport in semi-Dirac materials

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We show that a semi-Dirac (SD) system with an inversion symmetry breaking mass exhibits a topological phase transition when irradiated with off-resonant light. Using Floquet theory, we derive the band structure, Chern numbers, phase diagram, and we show that as the light intensity is swept at fixed mass, the SD system undergoes a normal-Chern-normal insulator transition. Along the phase boundaries, we observe single semi-Dirac-cone (SSDC) semimetal states in which one SD cone is gapless and the other is gapped. The nontrivial Berry curvature distribution $\Omega(\mathbf{k}) \neq -\Omega(-\mathbf{k})$ generates an orbital magnetization M and anomalous Nernst (α_{xy}) and thermal Hall (κ_{xy}) conductivities. We show that M remains constant as the Fermi level E_F scans the insulating gap, but it changes linearly with it in the Chern insulator (CI) phase, as expected. In the normal insulator phase, we find that α_{xy} exhibits a dip-peak profile that is reversed in the CI phase. We also find that switching the light's circular polarization from left to right induces a sign change in M , α_{xy} , and κ_{xy} , regardless of the topological phase, thereby allowing us to reverse the direction of flow of the transverse charge and heat currents. Further, we evaluate the components of the charge (σ_{aa}), thermoelectric (α_{aa}), and thermal (κ_{aa}) conductivity tensors ($a = x, y$) and examine the effect of light on them. With a linear dispersion along the y -direction, we find that α_{yy} and κ_{yy} are significantly larger than α_{xx} and κ_{xx} , respectively, due to the much larger squared Dirac velocity v_y^2 compared to v_x^2 .

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I. INTRODUCTION

The realization of topological insulator phases in Dirac materials and of their remarkable properties at their boundaries has been a major challenge [1,2]. For instance, the quantum anomalous Hall phase—also called a Chern insulator (CI), appears in lattice models with time-reversal symmetry (TRS) breaking Bloch bands carrying a finite Chern number [3] in the absence of a magnetic field. However, it has proved challenging to realize this phase experimentally [4]. Another topological phase, the quantum spin Hall insulator (QSHI), originates from spin-orbit coupling and the preservation of TRS [5–7].

Since most materials are intrinsically nontopological, different techniques have been proposed to induce topological phases in them. These include external stimuli, such as pressure [8], disorder [9,10], impurity doping [11], and heterostructuring combined with electrostatic gating and strain [1]. In the case of the QSHI obtained in materials with a

bulk gapped spectrum (e.g., HgTe/CdTe quantum wells), the thickness of the quantum well controls the phase transition [12,13]. However, most of these techniques require careful band-structure engineering and do not exhibit a high degree of controllability.

On the other hand, a time-periodic perturbation can be used to manipulate the (Floquet)-Bloch states via the drive frequency, amplitude, and polarization [14–30], thereby inducing or modifying the topological properties of the bands. In fact, it has been demonstrated that circularly polarized light with suitably chosen parameters opens a gap in semimetallic systems, allowing them to host gapless edge modes with topological characteristics [15,31,32].

Some of these exotic effects also appear in another class of two-dimensional (2D) systems, the semi-Dirac (SD) semimetals [33–35] formed with massless and massive dispersions along perpendicular directions. This type of dispersion was found in systems such as the honeycomb lattice in a magnetic field [36], TiO₂/V₂O₃ nanostructures [37], photonic crystals [38], surface states of topological insulators [39], phosphorus-based materials [40–42], and a polariton lattice [43], to name a few. SD materials are also promising candidates for valleytronic device applications [44]. The dynamic polarization function and plasmons [45], transport [46], and optical [47,48] properties in SD materials have also been investigated. It has also been shown that shining light on a semimetallic SD system opens a gap and induces a CI phase with nonzero Chern number [26]. However, the topological properties of irradiated SD systems in the presence of a mass term and the

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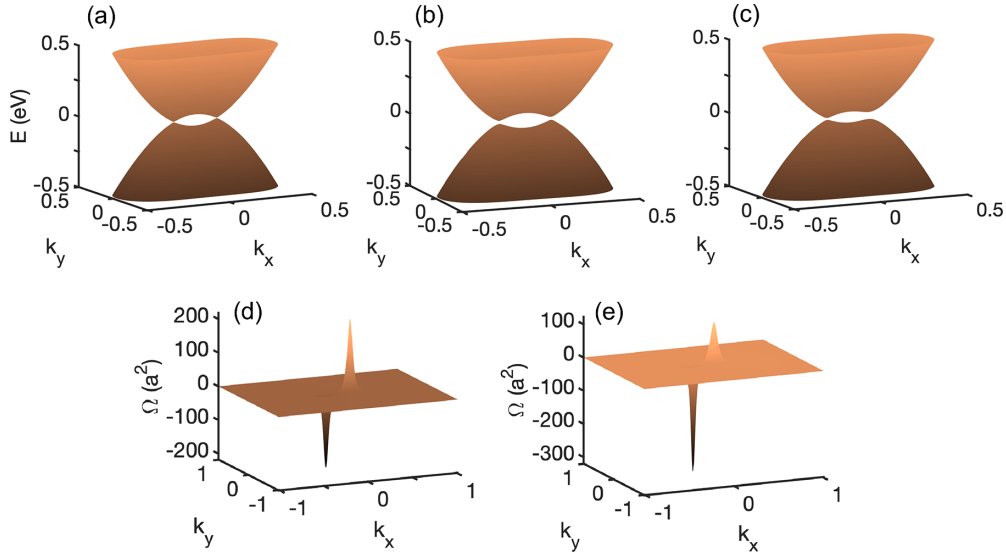


FIG. 1. (a)–(c) The energy spectrum of a SD material with a gap parameter $\Delta = -40$ meV. In (a) we plot the spectrum for $\tilde{A} = m = 0$; the system is semimetallic with two gapless SD nodes. In (b) $\tilde{A} = 0$ and $m = 10$ meV; the mass term gaps the SD nodes. The corresponding Berry curvature is shown in (d). It satisfies $\Omega(-\mathbf{k}) = -\Omega(\mathbf{k})$ due to the preservation of TRS. In (c) $\tilde{A} = 0.09 \text{ \AA}^{-1}$, $\omega = 3 \times 10^{15} \text{ Hz}$, and $m = 10$ meV; the simultaneous presence of light and mass generates different gaps at the two valleys. In this case, $\Omega(-\mathbf{k}) \neq -\Omega(\mathbf{k})$ as a consequence of the broken TRS; see (e).

consequences for the anomalous thermoelectric transport have not been explored so far.

The purpose of this work is twofold. First, using Floquet theory, we investigate the topological phase transition in a SD system, in the presence of an inversion symmetry breaking mass, irradiated with off-resonant light. When both light and mass are absent, the SD system is semimetallic with two SD nodes; see Fig. 1(a). The presence of the mass term alone opens a trivial gap; see Fig. 1(b). The application of light breaks TRS and opens a topological gap with $\Omega(-\mathbf{k}) \neq -\Omega(\mathbf{k})$ and a finite Chern number. The simultaneous presence of mass and light generates different gaps at the two valleys; see Fig. 1(c). In this case, we derive the phase diagram and show that, as the light intensity is swept at fixed mass, the SD system undergoes normal-Chern-normal insulator phase transitions. Along a phase boundary, single semi-Dirac-cone (SSDC) states appear, in which one SD cone is gapless and the other gapped; cf. Sec. III. We also investigate the fate of the CI phase at finite temperatures when the system is in a quantum mixed state described by a density matrix. We find that the CI phase survives for temperatures $\lesssim 30$ K for experimentally realizable parameters.

The nonzero local Berry curvature in irradiated SD materials induces anomalous transport responses, such as the anomalous Hall effect (AHE), the anomalous Nernst effect (ANE), and the anomalous thermal Hall effect (ATHE). It also generates an orbital magnetization (OM). Our second objective is to investigate these responses in the (normal) band insulator (BI) and CI phases. The OM, a quantity closely related to the ANE and AHE, remains constant as E_F scans the insulating gap, but it changes linearly with it in the CI phase. Importantly, we find that switching the light's circular polarization, from left to right, induces a sign change in M and the transverse conductivities σ_{xy} , α_{xy} , and κ_{xy} .

Further, we evaluate σ_{xx} and σ_{yy} and find analytical expressions for zero temperature when the spectrum exhibits a gapless SD point. We also find that the effect of light on α_{xx} is opposite to that on α_{yy} ; α_{xx} decreases with the light intensity whereas α_{yy} increases. The thermal conductivities κ_{xx} and κ_{yy} are also evaluated; they exhibit a behavior similar to those of σ_{xx} and σ_{yy} .

In Sec. II we derive an effective static (Floquet) Hamiltonian, the energy spectrum, and Berry curvature of an irradiated SD material with a mass term. In Sec. III we derive the Chern numbers, phase diagram, and discuss the phase transitions and the effect of temperature. The OM is evaluated in Sec. IV. In Sec. V we investigate the charge and thermoelectric transport and in Sec. VI we discuss potential optothermoelectric applications. We summarize and conclude in Sec. VII.

II. FLOQUET THEORY AND BERRY CURVATURE

We consider a SD material under the application of time-dependent radiation generated by an off-resonant polarized light field. The driven system is described by a time-periodic Hamiltonian $H(\mathbf{k}, t) = H(\mathbf{k}, t + T)$, where $T = 2\pi/\omega$ is the driving period and ω is the driving frequency. The time dependence of the electric field is induced via the electromagnetic vector potential, $\mathbf{A}(t) = (A_x(t), A_y(t))$, which is taken to be

$$\mathbf{A}(t) = A_0[\cos(\omega t)\hat{x} + \cos(\omega t - \phi)\hat{y}], \quad (1)$$

where ϕ allows tuning the light polarization and $A_0 = E_0/\omega$ is the driving amplitude, with E_0 the amplitude of the electric field $\mathbf{E} = -\partial\mathbf{A}/\partial t$. For $\phi = \pi/2$ ($-\pi/2$), the light is left (right) circularly polarized; for $\phi = 0$ and π it is linearly polarized.

The coupling to the electromagnetic field is introduced by replacing the momentum $\mathbf{p}$ with the covariant momentum

$\mathbf{p} - e\mathbf{A}(t)$, where $e < 0$ is the electron charge. We assume that the sample is smaller than the wavelength of light, so there is no spatial dependence of the driving field. Then the irradiated SD material is described by the time-dependent Bloch Hamiltonian

$$H(\mathbf{k}, t) = [\Delta + \alpha\pi_x^2(t)]\sigma_x + \gamma\pi_y(t)\sigma_y + m\sigma_z, \quad (2)$$

where $\pi_j(t) = k_j - (e/\hbar)A_j(t)$ with $j = x, y$; Δ is the gap parameter [49,50], m is the mass term, $\gamma = \hbar v_y$ with v_y the Dirac velocity along the y direction, $\alpha = \hbar^2/2m^*$ with m^* is the effective mass, associated with the x direction, and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices in the sublattice pseudospin space. We use $m^* \simeq 1.49m_e$, where m_e is the free-electron mass and $v_y \simeq 3 \times 10^5$ m/s, which are parameters relevant to monolayer black phosphorus [40].

In the irradiated SD material, a quantum state evolves as $|\psi_{\mathbf{k}}\rangle = U_{\mathbf{k}}(t, t_0)|\psi_{\mathbf{k}}(t, t_0)\rangle$, where $U_{\mathbf{k}}(t, t_0) = \mathcal{T} \exp(-(i/\hbar) \int_{t_0}^t H(\mathbf{k}, t') dt')$ is the time-evolution operator with $\mathcal{T}$ the time-ordering operator and t_0 is the initial time of the perturbation. For photon energies much larger than that of the electrons, $H(\mathbf{k}, t)$ can be reduced to an effective time-independent Hamiltonian using Floquet theory [31]. We define this Hamiltonian through the time-evolution operator over one period $U_{\mathbf{k}}(T, 0)$ as

$$\mathcal{T} \exp\left(-\frac{i}{\hbar} \int_0^T H(\mathbf{k}, t') dt'\right) = \exp\left(-\frac{i}{\hbar} H_F(\mathbf{k}) T\right), \quad (3)$$

where we have assumed $t_0 = 0$. A high-frequency expansion of $U_{\mathbf{k}}(T, 0)$, up to first order in inverse frequency, yields the Floquet Hamiltonian

$$H_F(\mathbf{k}) \simeq H_0 + \frac{[H_{-1}, H_{+1}]}{\hbar\omega}, \quad (4)$$

where $H_n = (1/T) \int_0^T e^{-in\omega t} H(\mathbf{k}, t) dt$ is the discrete Fourier component of the time-periodic Hamiltonian $H(\mathbf{k}, t)$. This approach is valid for high frequencies and low intensities, such that $eA_0 v_y \ll \hbar\omega$. The off-resonant light does not excite electrons, and there is no optical absorption. Instead, it modifies the electron band structure through second-order virtual photon absorption processes that lead to the creation or modification of the band gap [31,32].

Using Eqs. (2)–(4), we obtain

$$H_0 = \left(\Delta + \alpha k_x^2 + \frac{\alpha e^2 A_0^2}{2\hbar^2} \right) \sigma_x + \gamma k_y \sigma_y + m \sigma_z \quad (5)$$

and

$$H_{\pm 1} = -\frac{1}{\hbar} \alpha e A_0 k_x \sigma_x - \frac{1}{2} e A_0 v_y e^{\mp i\phi} \sigma_y. \quad (6)$$

Evaluating the commutator in Eq. (4) gives $[H_{-1}, H_{+1}] = \hbar\omega\eta k_x \sigma_z$, where $\eta = 2\alpha v_y \tilde{A}^2 \sin\phi/\omega$ with $\tilde{A} = eA_0/\hbar$. Then the Floquet Hamiltonian reads

$$H_F(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (7)$$

where

$$\mathbf{d}(\mathbf{k}) = (\Delta_1 + \alpha k_x^2, \gamma k_y, m_z), \quad (8)$$

with $\Delta_1 = \Delta + \alpha\tilde{A}^2/2$ and $m_z = m + \eta k_x$. The energy dispersion, obtained by squaring the Hamiltonian, is $E_{\mathbf{k}} = \sqrt{\mathbf{d}(\mathbf{k}) \cdot \mathbf{d}(\mathbf{k})} = \lambda \varepsilon_{\mathbf{k}}$, with $\lambda = +1(-1)$ for the conduction

(valence) band and

$$\varepsilon_{\mathbf{k}} = [(\Delta_1 + \alpha k_x^2)^2 + \gamma^2 k_y^2 + (m + \eta k_x)^2]^{1/2}. \quad (9)$$

In the above model, the light-induced term $h(\mathbf{k}) = \eta k_x \sigma_z$ breaks TRS; explicitly, $\Theta h(\mathbf{k}) \Theta^{-1} \neq h(-\mathbf{k})$, with $\Theta = \mathcal{K}$ the complex conjugation operator. For linearly polarized light ($\phi = 0, \pi$), for which $\eta = 0$, TRS is preserved.

In Figs. 1(a)–1(c) we show the energy dispersion $E_{\mathbf{k}}$ as a function of $\mathbf{k}$ for $\Delta = -40$ meV. In Fig. 1(a), $\tilde{A} = m = 0$, the system is in the semimetallic state with two gapless SD nodes located at $\mathbf{k}_D^{\pm} = (\pm\sqrt{-\Delta/\alpha}, 0)$ [51]. In Fig. 1(b), $\tilde{A} = 0$ and $m = 10$ meV, TRS is preserved and the band gap is trivial. The Berry curvature evaluated in Eq. (11) is shown in Fig. 1(d). The spectrum under the application of light and in the presence of mass is shown in Fig. 1(c) and the Berry curvature in Fig. 1(e) for $\tilde{A} = 0.09 \text{ \AA}^{-1}$, $\omega = 3 \times 10^{15} \text{ Hz}$, and $m = 10$ meV. In this case, $\Delta_1 < 0$, the light gaps the SD nodes and shifts their positions at $\mathbf{k}_D^{\pm} = (k_D^{\pm}, 0)$ with $k_D^{\pm} = \pm\sqrt{-\Delta_1/\alpha}$ [52]. As will be shown below, when $\Delta_1 < 0$ the system is a CI for $|m| < |\eta k_D|$ and a BI for $|m| > |\eta k_D|$. We remark that for $\Delta_1 = 0$, i.e., for $\Delta = -\alpha\tilde{A}^2/2$, it is evident from Eq. (9) that the spectrum exhibits a gapless (gapped) SD point for $m = 0$ ($m \neq 0$). For $\Delta_1 > 0$, the system is a BI regardless of the value of m , as will be shown later.

Berry curvature. For the above two-band model, the Berry curvature can be expressed as [1]

$$\Omega(\mathbf{k}) = \frac{1}{2|\mathbf{d}|^3} \mathbf{d} \cdot (\partial_{k_x} \mathbf{d} \times \partial_{k_y} \mathbf{d}). \quad (10)$$

Using $\mathbf{d}(\mathbf{k})$ from Eq. (8), we get

$$\Omega(\mathbf{k}) = \frac{\gamma\eta(\alpha k_x^2 - \Delta_1) + 2\alpha\gamma m k_x}{2\varepsilon_{\mathbf{k}}^3}. \quad (11)$$

In the absence of light, $\eta = 0$, Eq. (11) satisfies $\Omega(-\mathbf{k}) = -\Omega(\mathbf{k})$. Under the application of light, $\eta \neq 0$, it satisfies $\Omega(-\mathbf{k}) \neq -\Omega(\mathbf{k})$.

III. CHERN NUMBERS AND TOPOLOGICAL TRANSITION

We characterize the topology of the irradiated SD system by explicitly calculating the Chern numbers. We employ the method of the Brouwer degree [53] in order to evaluate the Chern number as

$$\mathcal{C} = \frac{1}{2} \sum_{\mathbf{k} \in \mathbf{D}_i} \text{sgn}(J_z)_i \text{sgn}(d_z)_i, \quad (12)$$

where $J_z = \partial_{k_x} d_x \partial_{k_y} d_y - \partial_{k_y} d_y \partial_{k_x} d_x$ is the Jacobian, and $\text{sgn}(x)$ is the sign function. In this approach, instead of integrating the Berry curvature in the Brillouin zone, we need to evaluate a discrete sum over the momenta $\mathbf{k}$ in the set of Dirac points $\mathbf{D}_i$. The Jacobian is found to be $J_z = 2\alpha\gamma k_x$; at the Dirac points, $\text{sgn}[J_z(\mathbf{k}_D^{\pm})] = \pm 1$, which also gives their chirality. The sign of the mass term at the Dirac points is expressed as $\text{sgn}[m_z(\mathbf{k}_D^{\pm})] = \text{sgn}(m \pm \eta k_D)$ with $k_D = |k_D^+| = |k_D^-|$. Thus the Chern number reads

$$\mathcal{C} = \frac{1}{2} [\text{sgn}(m + |\eta|k_D) - \text{sgn}(m - |\eta|k_D)]. \quad (13)$$

Assuming the polarization of light is $0 < \phi < \pi$ ($\eta > 0$), we find $\mathcal{C} = 0$ for $m > \eta k_D$; the mass term has the same sign at

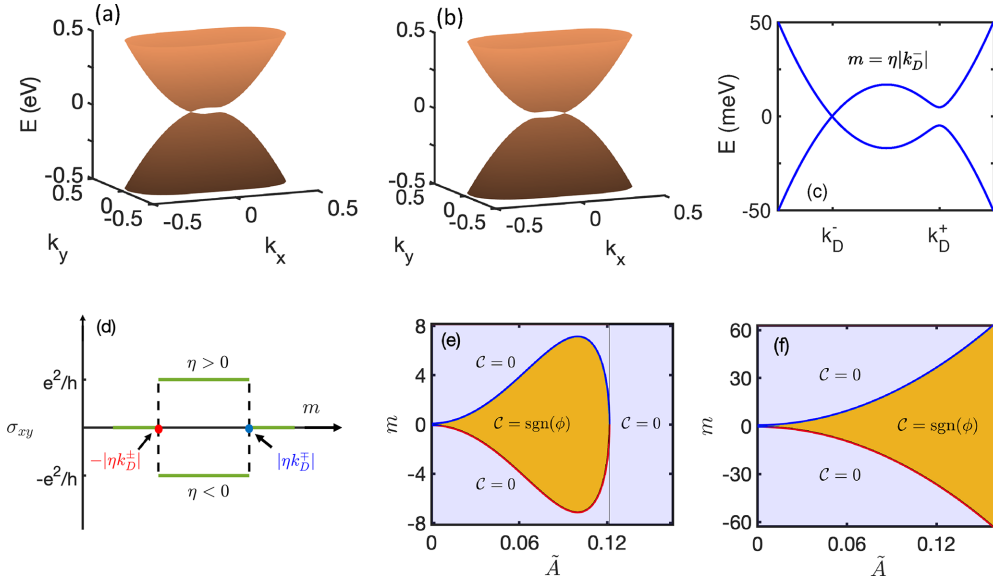


FIG. 2. (a),(b) The band structure of a SD material in the SSDC semimetal states at the phase transition points (a) $m = \eta k_D$ and (b) $m = -\eta k_D$. The parameter values are $\Delta = -20$ meV, $\tilde{A} = 0.09 \text{ \AA}^{-1}$, $\omega = 3 \times 10^{15}$ Hz, and $\phi = \pi/2$. In (a) the gap is open at k_D^+ but closed at k_D^- with linear dispersion along k_y . (c) The band structure of (a) for $k_y = 0$ showing the SSDC state. (d) σ_{xy} vs m for both left- and right-circularly polarized light. (e) $(m, \tilde{A})$ phase diagram. The thin vertical line at $\tilde{A}_{th} \simeq 0.12 \text{ \AA}^{-1}$ corresponds to $\Delta_1 = 0$. (f) $(m, \tilde{A})$ phase diagram for an isotropic model with linear bands.

the Dirac points. As m decreases (or as the light intensity increases), the Dirac node at k_D^- goes through a gap closing and opening transition at $m = \eta|k_D^-|$; the gap at the second Dirac node stays open, see Fig. 2(a). For $-\eta k_D < m < \eta k_D$ we find $C = 1$; the SD system is in the CI phase. As m further decreases, the second Dirac node undergoes a gap closing and opening transition at $m = -\eta k_D^+$; the first Dirac node remains gapped; see Fig. 2(b). For $m < -\eta k_D$, the system is a BI with $C = 0$. When the polarization is $-\pi < \phi < 0$ ($\eta < 0$), the order of the gap closings is reversed. In this case, we find $C = -1$ for $-\eta|k_D < m < \eta|k_D$, and $C = 0$ otherwise. These results can be expressed as

$$C = \begin{cases} \text{sgn}(\phi), & |m| < |\eta|k_D, \\ 0, & |m| > |\eta|k_D. \end{cases} \quad (14)$$

The SSDC states appear at the phase transition points, $|m| = |\eta|k_D$, where only one SD cone is gapless and the other one is gapped. In Fig. 2(c) the SSDC state is shown for $m = \eta|k_D^-|$; it was obtained from the band structure of Fig. 2(a) by plotting $E_{\lambda\mathbf{k}}$ versus k_x for $k_y = 0$. These remarkable states can only be realized when light and mass are simultaneously present. They were found previously in photoirradiated silicene [54] and recently in jacutingaite [55] without the application of light but with broken inversion and TRS.

In Fig. 2(d) we show the Hall conductivity σ_{xy} as a function of the mass m for $\eta > 0$ and $\eta < 0$. For $|m| < |\eta|k_D$, $\sigma_{xy} = (e^2/h)\text{sgn}(\eta)$; $\sigma_{xy} = 0$ otherwise. At the phase transition points, σ_{xy} jumps from 0 to $\pm e^2/h$.

In Fig. 2(e) we show the $(m, \tilde{A})$ phase diagram. The blue (red) line corresponds to the gap closing and opening at $|k_D^-|$ (k_D^+) for $\eta > 0$; for $\eta < 0$ they are swapped. These lines correspond to the SSDC states. We notice that the SD system undergoes a normal-Chern-normal insulator phase transition as the light intensity increases from zero at a fixed value of

the mass. As $\tilde{A}$ approaches the threshold value $\tilde{A}_{th} \simeq 0.12 \text{ \AA}^{-1}$ for which $\Delta_1 \rightarrow 0$ [see the thin vertical line in Fig. 2(e)], the SSDC state gradually shifts and becomes a SD node at $\mathbf{k}_D = 0$. For $\tilde{A} > \tilde{A}_{th}$ so that $\Delta_1 > 0$, the SD node is gapped; in this case, the system is a BI with $C = 0$ [56]. These transitions also occur when varying m at a fixed value of $\tilde{A}$. We emphasize here that for $m = 0$, there are no SSDC states and the gaps are the same at the two valleys; in this case, $C = \text{sgn}(\phi)$ for $\Delta_1 < 0$ and $C = 0$ for $\Delta_1 > 0$ [26].

Comparison with isotropic Dirac systems. It is instructive to make a comparison with light-induced topological transitions in isotropic Dirac systems possessing linear bands. A prototype Dirac system is the honeycomb lattice (for example, monolayer graphene), whose low-energy Hamiltonian is given by

$$H_g(\mathbf{k}) = \hbar v_F (\tau_z \sigma_x k_x + \sigma_y k_y) + m \sigma_z, \quad (15)$$

where $\tau_z = \pm 1$ is the valley pseudospin for the K and $K' = -K$ valleys. We have included an inversion symmetry breaking mass m originating from a site energy difference $2m$ between sublattices. When irradiated with off-resonant light, we can use the vector potential in Eq. (1) and the Floquet approach to obtain an effective time-independent Hamiltonian

$$H_F^g(\mathbf{k}) = \mathbf{d}_g(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (16)$$

where

$$\mathbf{d}_g(\mathbf{k}) = (\hbar v_F \tau_z k_x, \hbar v_F k_y, m_g), \quad (17)$$

with $m_g = m + \eta' \tau_z$ and $\eta' = \hbar^2 v_F^2 \tilde{A}^2 \sin \phi / \omega$. The energy dispersion is given by $E_{\lambda\mathbf{k}} = \lambda \varepsilon_{\mathbf{k}}'$ with $\varepsilon_{\mathbf{k}}' = (\hbar^2 v_F^2 k^2 + m_g^2)^{1/2}$. The light-induced term $\hbar \tau_z(\mathbf{k}) = \eta' \tau_z \sigma_z$ is of the Haldane type and breaks TRS; explicitly, $\Theta \hbar \tau_z(\mathbf{k}) \Theta^{-1} \neq \hbar \tau_z(-\mathbf{k})$, with $\Theta = \tau_x \mathcal{K}$. For $\eta' > 0$, this term is negative at K' and positive at

K ; the edge states will connect one Dirac cone with another by crossing the gap [57]. The light-induced term in SD systems, $h(\mathbf{k}) = \eta k_x \sigma_z$, is negative (positive) at $k_x = -k_D (+k_D)$ and the behavior of the edge states will be similar.

To evaluate the Chern number, we need the sign of the Jacobian at the Dirac points $\mathbf{k}_D^\pm = \pm \mathbf{K}$. We find $J_z = \hbar^2 v_F^2 \tau_z$ and at the Dirac points $\text{sgn}[J_z(\mathbf{k}_D^\pm)] = \pm 1$. The mass sign at the Dirac points is $\text{sgn}[m_g(\mathbf{k}_D^\pm)] = \text{sgn}(m \pm \eta')$. Thus the Chern number reads

$$C = \frac{1}{2} [\text{sgn}(m + |\eta'|) - \text{sgn}(m - |\eta'|)]. \quad (18)$$

As m varies, we obtain gap closing and reopening transitions at $m = \pm |\eta'|$ similarly to SD systems; the mass term vanishes at one Dirac point, $m + \eta' \tau_z = 0$. For $m = \eta'$ the Dirac cone at K' is gapless and at K it is gapped. For $m = -\eta'$ they are swapped.

However, there is an important difference between the Chern numbers in Eqs. (13) and (18). An isotropic Dirac system remains gapped with $C = \text{sgn}(\phi)$ regardless of the light intensity $\tilde{A}$ as long as $|m| < |\eta'|$. This is shown in the $(m, \tilde{A})$ phase diagram in Fig. 2(f). The blue (red) line corresponds to the gap closing at the K' (K) valley for $\eta' > 0$; for $\eta' < 0$ they are swapped. The Dirac system undergoes a normal-to-Chern-insulator phase transition as $\tilde{A}$ increases from zero; one can traverse the phase boundary between the regions with $C = 0$ and $C = \text{sgn}(\phi)$ only once. This is in contrast to a SD system, which undergoes a normal-Chern-normal phase transition as $\tilde{A}$ increases from zero. As $\tilde{A}$ reaches $\tilde{A}_{\text{th}}$ ($\Delta_1 \rightarrow 0$) the topological gap closes and reopens with $C = 0$; one can traverse the phase boundary twice; see Fig. 2(e). This is due to the presence of k_x in the mass term m_z in Eq. (8), which becomes k_D in the Chern number in Eq. (13).

Anomalous Hall conductivity. Using the Berry curvature from Eq. (11), we evaluate the anomalous Hall conductivity as

$$\sigma_{xy} = \frac{e^2}{h} \int \frac{d^2 k}{(2\pi)^2} (f_{-\mathbf{k}} - f_{+\mathbf{k}}) \Omega(\mathbf{k}), \quad (19)$$

where $f_{\pm \mathbf{k}} = \{1 + \exp[\beta(\pm \varepsilon_{\mathbf{k}} - E_F)]\}^{-1}$ is the Fermi distribution function of the conduction (+) and valence (−) bands and $\beta = 1/k_B T$ with k_B the Boltzmann constant and T the temperature. In Fig. 3 we show numerical results of σ_{xy} versus E_F for left-circularly polarized light ($\phi = \pi/2$) and $T = 0.1$ K. We have used $\Delta = -20$ meV, $\omega = 3 \times 10^{15}$ Hz, and $m = 2.5$ meV. The values of $\tilde{A}$ are such that $\Delta_1 < 0$ in both Figs. 3(a) and 3(b) [58]. In Fig. 3(a) we observe that σ_{xy} is finite and quantized for E_F in the gap; it is in the CI phase. As the light intensity decreases, the energy gap gradually shrinks and brings the system to an SSDC state where the gap closes at $|m| = |\eta|k_D$. It then reopens for $|m| > |\eta|k_D$, and a further decrease of the light intensity $\tilde{A}$ causes the AHC to vanish inside the gap, as shown in Fig. 3(b). Thus the interplay of light and mass (see Ref. [60] and Appendix) offers the possibility to change the topological phase. We also notice that, away from the gap, the Hall conductivity is small. This is due to the small value of η for weak light intensity $\tilde{A}$.

In Fig. 3(c) we show σ_{xy} versus E_F in the CI phase for left- and right-circularly polarized light, $\phi = \pi/2$ and $-\pi/2$, respectively. We notice that σ_{xy} is reversed when switching the

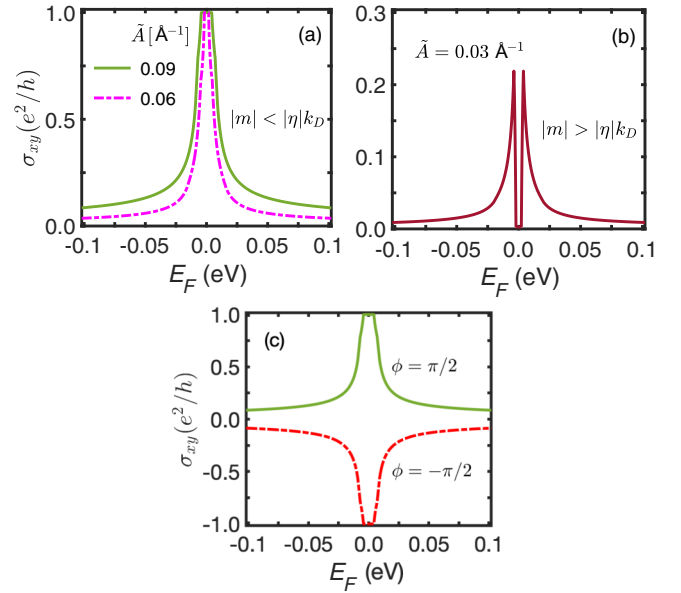


FIG. 3. (a),(b) Anomalous Hall conductivity σ_{xy} as a function of E_F for $\Delta_1 < 0$. In (a) the SD system is a CI with $\sigma_{xy} = e^2/h$ for E_F in the gap and in (b) it is a BI with $\sigma_{xy} = 0$; the topological phase transition occurs at $m = |\eta|k_D$. (c) σ_{xy} vs E_F for left- and right-circularly polarized light in the CI phase.

polarization of light indicating that the direction of the edge state is reversed; this is also evident from Eq. (14).

Temperature effects on the CI phase. Chern invariants for systems with broken TRS lead to quantized Hall conductivities at temperatures well below the energy gap. However, at finite temperatures, quantization is lost due to thermal averaging or dephasing to mixed states [61–65]. This issue has led to the question of a proper definition of a topological invariant for a mixed rather than a pure state. The extension of the Chern invariant based on the density matrix for mixed states is rather nontrivial, and no universally agreed upon definition exists. Here, we employ the mean Uhlmann curvature (MUC) [66] to evaluate the thermal Uhlmann number.

In thermal equilibrium, the state of the system is described by the density operator $\rho = e^{-\beta H_F} / \mathcal{Z}$, where $\mathcal{Z} = \text{tr}(e^{-\beta H_F})$ is the partition function, with H_F given in Eq. (7); it can be readily evaluated to give $\mathcal{Z} = 2 \cosh(\beta|\mathbf{d}|)$. For a two-band model, the MUC, which is a mixed state generalization of the Berry curvature, is given as [65,66]

$$\mathcal{U}(\mathbf{k}, T) = \frac{\tanh^3(\beta|\mathbf{d}|)}{2|\mathbf{d}|^3} \mathbf{d} \cdot (\partial_{kx} \mathbf{d} \times \partial_{ky} \mathbf{d}). \quad (20)$$

In the limit $T \rightarrow 0$, $\mathcal{U}(\mathbf{k}, T)$ reduces to the Berry curvature in Eq. (10). For $T \rightarrow \infty$ it vanishes; the valence and conduction bands are equally populated in this limit, but they contribute with opposite curvatures. In a continuum model Hamiltonian, the Uhlmann number is calculated by integrating the MUC in the entire momentum space:

$$n_U = \frac{1}{2\pi} \int \mathcal{U}(\mathbf{k}, T) d^2 k. \quad (21)$$

In Fig. 4(a) we show n_U as a function of temperature T for E_F placed in the middle of the gap. The values of the

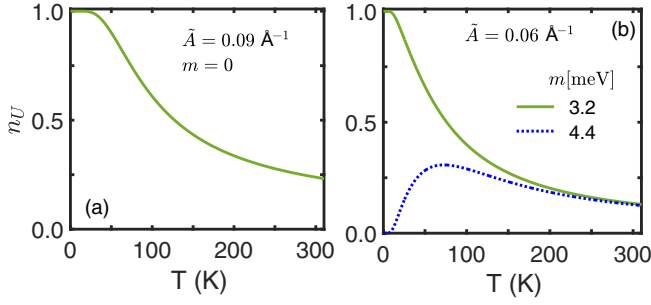


FIG. 4. (a) Thermal Uhlmann number n_U as a function of temperature T . The system is a CI with $n_U = 1$ for $T < T_c$ with $T_c \simeq 30$ K. For these values of m and $\tilde{A}$ the system is away from the phase boundaries; see Fig. 2(e). (b) The same as in (a), but the values of m are such that the system is just below ($m = 3.2$ meV) or just above ($m = 4.4$ meV) the phase transition.

light intensity and of the mass are such that the system is in the CI phase for $T = 0$; it is inside the topological region in Fig. 2(e). Notice that for $T = 0$, n_U correctly reproduces the Chern number result. The system remains in the CI phase, $n_U = 1$, even at nonzero temperature, provided that it is below a certain critical T_c associated with the band gap. For the chosen parameters, n_U starts losing its quantized value at $T_c \simeq 30$ K for which $k_B T \simeq 2.6$ meV. This is comparable to the band gap ($\simeq 5$ meV). It is reasonable to expect that, for a larger topological gap, the CI phase remains stable ($n_U = 1$) for larger T_c .

However, when the system approaches a topological transition point at the blue (or red) line in Fig. 2(e), it is expected that the CI phase becomes less stable. This is illustrated in Fig. 4(b), where we show n_U versus T for $\tilde{A} = 0.06 \text{ \AA}^{-1}$. We have used two values of the mass, $m = 3.2$ and 4.4 meV, which correspond to points just below and just above the topological transition at $m = |\eta|k_D \simeq 3.8$ meV. We notice that for $m = 3.2$ meV, n_U starts decreasing from unity much sooner ($T_c \simeq 8$ K); the gap is $\simeq 2$ meV in this case. On the other hand, for $m = 4.4$ meV, the system is a BI [i.e., it is outside the topological region in the $(m, \tilde{A})$ phase diagram] for which $n_U = 0$ at $T = 0$. For finite T , n_U becomes nonzero, which is attributed to thermal activation and partial filling of the conduction band. In the limit $T \rightarrow \infty$, the conduction band has equal population with the valence band, but the curvatures have opposite sign yielding $n_U \rightarrow 0$.

IV. ORBITAL MAGNETIZATION

The TRS breaking light can generate finite OM, a quantity closely related to anomalous thermoelectric transport. In fact, it is the Berry phase correction to the OM that leads to the ANE [67]. The OM has been investigated in various systems, such as transition-metal dichalcogenides [68,69], topological insulators [25], and Weyl semimetals [70], to name a few. We obtain the OM from the free energy F in a weak magnetic field $\mathbf{B}$ written as

$$F = -\frac{1}{\beta} \sum_{\lambda\mathbf{k}} \ln[1 + e^{-\beta(E_M - E_F)}], \quad (22)$$

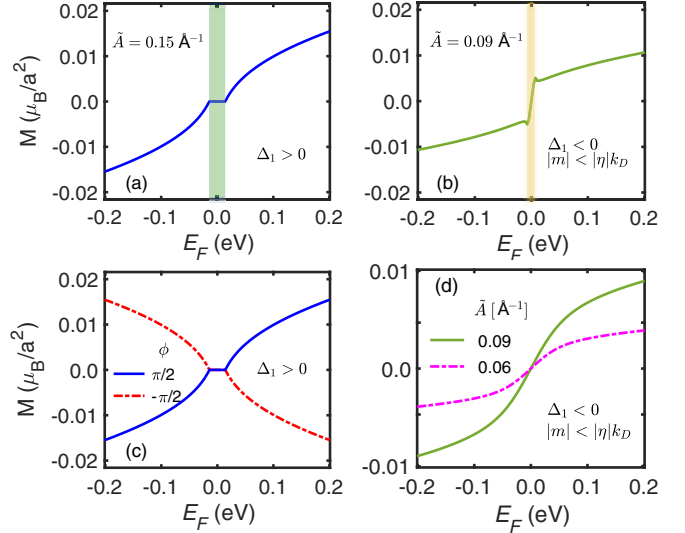


FIG. 5. Orbital magnetization M as a function of the chemical potential E_F for an irradiated SD system in the (a) BI and (b) CI phase for $T = 0.1$ K. (c) M as a function of E_F in the BI phase for left- and right-circularly polarized light shown by the blue (solid) and red (dashed-dotted) lines, respectively. (d) M as a function of E_F in the CI phase for $T = 300$ K.

where the electron energy $E_M = E_{\lambda\mathbf{k}} - \mathbf{m}(\mathbf{k}) \cdot \mathbf{B}$ includes a correction due to the orbital magnetic moment $\mathbf{m}(\mathbf{k})$. The OM of a band is given by $M_\lambda = -(\partial F / \partial B)_{E_F, T} = M_\lambda^{(o)} + M_\lambda^{(b)}$, where

$$M_\lambda^{(o)} = \frac{a^2}{(2\pi)^2} \int d^2k f_{\lambda\mathbf{k}} m_\lambda(\mathbf{k}), \quad (23)$$

$$M_\lambda^{(b)} = \frac{ea^2}{2\pi\beta\hbar} \int d^2k \Omega_\lambda(\mathbf{k}) \ln[1 + e^{-\beta(E_{\lambda\mathbf{k}} - E_F)}], \quad (24)$$

where $a = 3.3 \text{ \AA}$ is the lattice constant [40]. $M_\lambda^{(o)}$ is due to the thermodynamic average of the magnetic moments, whereas $M_\lambda^{(b)}$ results from the Berry phase correction to the electron density of states [67]. The OM is given as $M = \sum_\lambda M_\lambda$. For a two-band model with particle-hole symmetry, the orbital magnetic moment and Berry curvature are related by $\mathbf{m}_\lambda(\mathbf{k}) = (e/2\hbar)(E_\lambda - E_{\lambda'})\boldsymbol{\Omega}_\lambda(\mathbf{k})$ [71]. Using this relation, the OM at zero temperature can be simplified to

$$M_\lambda = (1/e)E_F\sigma_{xy}. \quad (25)$$

This relation is understood by the fact that the Hall conductivity is equal to the derivative of the OM with respect to the chemical potential E_F [72]. When the chemical potential varies in the insulating gap, the OM changes linearly if the Chern number is nonzero; it remains constant otherwise.

In Figs. 5(a) and 5(b), we show the OM M versus the chemical potential E_F in the BI and CI phase, respectively, for $\phi = \pi/2$ and $T = 0.1$ K, in units of μ_B/a^2 , where $\mu_B = e\hbar/2m^*$ is the Bohr magneton. In this and the next section, the BI phase corresponds to $\Delta_1 > 0$ and CI to $\Delta_1 < 0$ with $|m| < |\eta|k_D$. We have used $\Delta = -15$ meV, $\omega = 3 \times 10^{15}$ Hz, and $m = 2$ meV. The values $\tilde{A} = 0.15 \text{ \AA}^{-1}$ and $0.09 \text{ \AA}^{-1}$ ensure that the SD system is a BI and CI, respectively. The shaded areas show the band gaps in the two cases. In the CI

phase, the SD system carries a dissipationless chiral edge state that contributes to the OM. The linearity of M on E_F can be seen as the effect of populating the edge state. In the BI phase, we notice that the OM is constant in the gap, in accordance with Eq. (25).

In Fig. 5(c) we show M versus E_F in the BI phase for left- and right-circularly polarized light, for the same parameter values as in Fig. 5(a). Notice that switching the light polarization induces a reversal of M . In Fig. 5(d) we show M versus E_F in the CI phase for $T = 300$ K and for two values of $\tilde{A}$. We notice that the linear behavior of M in the gap is smoothed out due to the Fermi distributions. We also note that the values of M become smaller as the light intensity decreases.

V. CHARGE AND THERMOELECTRIC TRANSPORT

In the presence of an electric field $\mathbf{E}$ and a temperature gradient ∇T , the charge current $\mathbf{J}$ and heat current $\mathbf{J}_Q$ are determined through the following linear-response equations:

$$\begin{pmatrix} \mathbf{J} \\ \mathbf{J}_Q \end{pmatrix} = \begin{pmatrix} \sigma & \alpha \\ T\alpha & \kappa \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ -\nabla T \end{pmatrix}, \quad (26)$$

where σ , α , and κ are the charge, thermoelectric, and thermal conductivity tensors, respectively. The off-diagonal (anomalous) components σ_{xy} have been evaluated and discussed in the context of the topological phase transition in Sec. III. In this section, we evaluate the diagonal components σ_{aa} , α_{aa} , and κ_{aa} using the semiclassical Boltzmann treatment, as well as the off-diagonal components α_{ab} and κ_{ab} . We start with the latter two, which are known as anomalous Nernst and anomalous thermal Hall conductivities; they are topological thermoelectric responses because they arise from a finite Berry curvature.

A. Anomalous Nernst effect

The conventional Nernst effect [73] occurs in the presence of a longitudinal temperature gradient and an external magnetic field, which generates a transverse current $J_i = \alpha_{ij}(-\nabla_j T)$. A nontrivial Berry curvature also gives rise to a Nernst response, as a result of the anomalous velocity, leading to the ANE. It has been studied in various 2D and Dirac materials [30,69,73–76]. The ANE is the thermoelectric counterpart of the AHE.

The anomalous Nernst response to a temperature gradient can be obtained using the semiclassical wave-packet method together with the contribution of the orbital magnetization [67]. In this approach, the anomalous Nernst conductivity (ANC) α_{xy} is given as

$$\alpha_{xy} = \frac{ek_B}{\hbar} \sum_{\lambda} \int \frac{d^2k}{(2\pi)^2} \Omega_{\lambda}(\mathbf{k}) S_{\lambda}, \quad (27)$$

where $S_{\lambda}(\mathbf{k}) = -f_{\lambda\mathbf{k}} \ln f_{\lambda\mathbf{k}} - (1 - f_{\lambda\mathbf{k}}) \ln(1 - f_{\lambda\mathbf{k}})$ is the entropy density. $S_{\lambda}(\mathbf{k})$ vanishes for completely filled and completely empty bands, which implies that α_{xy} is a Fermi surface property. At low temperatures, the ANC is related to the zero-temperature Hall conductivity σ_{xy} through the Mott relation [77]

$$\alpha_{xy} = -\frac{\pi^2 k_B^2 T}{3e} \frac{d\sigma_{xy}}{dE_F}. \quad (28)$$

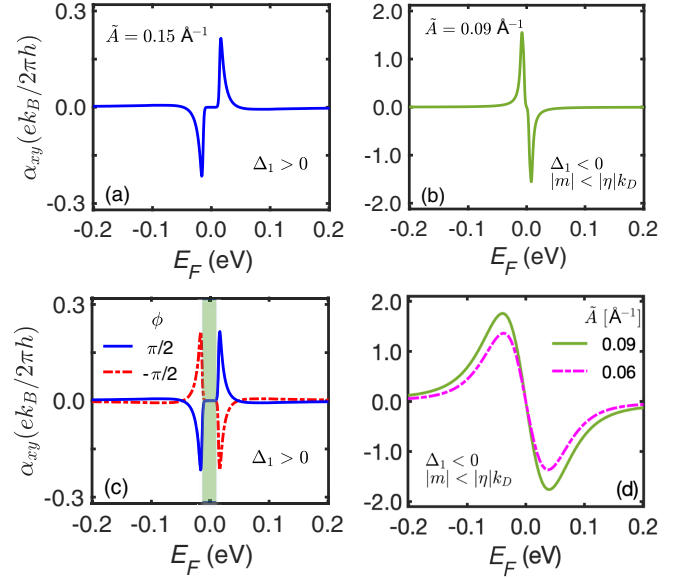


FIG. 6. ANC α_{xy} vs E_F for an irradiated SD system in the (a) BI and (b) CI phase for $T = 10$ K. (c) α_{xy} vs E_F in the BI phase for left- and right-circularly polarized light shown by the blue (solid) and red (dashed-dotted) lines, respectively. (d) α_{xy} vs E_F in the CI phase for $T = 300$ K.

The ANC versus the chemical potential is plotted in Figs. 6(a) and 6(b) for the BI and CI phase, respectively, for $\phi = \pi/2$ and $T = 10$ K. We have used the same parameter values as in Fig. 5. In Fig. 6(a) we notice that $\alpha_{xy} = 0$ when E_F is in the band gap, whereas at the band edges it exhibits a step jump. This can be understood from the Mott relation; for E_F in the gap, σ_{xy} is constant (see Fig. 3) and thus $d\sigma_{xy}/dE_F = 0$. At the band edges, $d\sigma_{xy}/dE_F$ is discontinuous, resulting in the sharp dip or peak in α_{xy} . Their opposite signs reflect those of the Berry curvatures of the respective bands. As E_F shifts away from the band edges, α_{xy} decays rapidly and eventually goes to zero; the magnitude of the Berry curvature decreases for electron or hole states away from the SD nodes. We verified numerically that the decay follows $\sim 1/E_F^2$.

In Fig. 6(b), α_{xy} exhibits approximately a 10-fold increase. This is a consequence of the value of the light intensity; it shrinks the band gap and brings the system close to an SSDC state, resulting in significantly enhanced Berry curvature. We also notice that the dip-peak profile is reversed compared to the BI phase; it is a consequence of the sign reversal in the Berry curvature for $\Delta_1 < 0$.

In Fig. 6(c) we show the ANC in the BI phase for left- and right-circularly polarized light. The parameter values are the same as in Fig. 6(a). We notice that switching the polarization of light induces a reversal of α_{xy} . This effect can also be observed in the CI phase. Thus the light polarization can be used to reverse the direction of transverse flow of thermoelectric charge current in a SD material. The effect of temperature is shown in Fig. 6(d), where we plot α_{xy} versus E_F for $T = 300$ K. We notice that the sharp jumps shown in Fig. 6(b) are smoothed out at high temperatures. At the peak we estimate $\alpha_{xy} \simeq 1$ nA/K, which is an order of magnitude larger than that of transition-metal dichalcogenides [69,74,75]

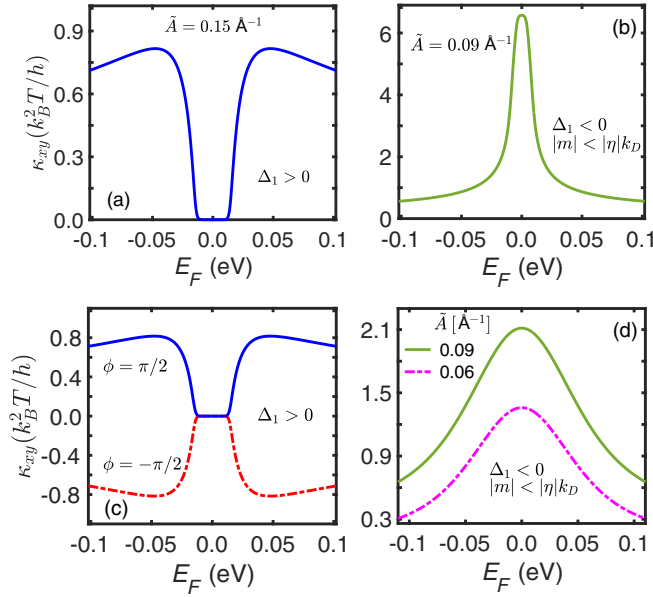


FIG. 7. ATHC κ_{xy} vs E_F for an irradiated SD system in the (a) BI and (b) CI phase for $T = 10$ K. (c) κ_{xy} vs E_F in the BI phase for left- and right-circularly polarized light shown by the blue (solid) and red (dashed-dotted) lines, respectively. (d) κ_{xy} vs E_F in the CI phase for $T = 200$ K.

and of strained graphene [73], partly because of the larger values of the Berry curvature. However, it is comparable to that of silicene [78] and jacutingaite [76].

B. Anomalous thermal Hall effect

The thermal Hall effect occurs in the presence of a temperature gradient in the longitudinal direction and an out-of-plane magnetic field, which generates a heat current in the transverse direction, $J_{Q,i} = \kappa_{ij}(-\nabla_j T)$ [79]. However, as in the Nernst effect, a nontrivial Berry curvature can play the role of a magnetic field, leading to the anomalous thermal Hall effect (ATHE).

The anomalous thermal Hall conductivity (ATHC) κ_{xy} is given by

$$\kappa_{xy} = \frac{k_B^2 T}{4\pi^2 \hbar} \sum_{\lambda} \int d^2 k \Omega_{\lambda}(\mathbf{k}) \left\{ \frac{\pi^2}{3} + \beta^2 (E - E_F)^2 f_{\lambda\mathbf{k}} - 2\text{Li}_2(1 - f_{\lambda\mathbf{k}}) - [\ln(1 - f_{\lambda\mathbf{k}})]^2 \right\}, \quad (29)$$

where $\text{Li}_n(z) = \sum_{k=1}^{\infty} z^k/k^n$ is the polylogarithmic function. At low temperatures the ATHC is related to the zero-temperature Hall conductivity σ_{xy} through the Wiedemann-Franz law [80] $\kappa_{xy} = (\pi^2 k_B^2 T/3e^2) \sigma_{xy}$. This relation indicates that κ_{xy} exhibits similar behavior to σ_{xy} ; they differ only by a factor.

In Figs. 7(a) and 7(b) we show κ_{xy} versus E_F evaluated using Eq. (29) for the BI and CI phase, respectively, for $\phi = \pi/2$ and $T = 10$ K. The parameter values are the same as in Fig. 6. We notice that in the BI phase, the ATHC vanishes when E_F is inside the gap. In the CI phase, κ_{xy} increases drastically and exhibits a much narrower plateau. In this case,

the system is near a SSDC state, i.e., near a band crossing, which generates enhanced Berry curvature, which then gives a large contribution to κ_{xy} .

In Fig. 7(c) we show the ATHC in the BI phase for left- and right-circular polarizations. As in the ANE, we notice that switching the polarization of the incident light from left- to right-circular induces a reversal of κ_{xy} . Thus the consequence of switching the polarization manifests as a reversal of heat flow. Such a reversal of heat flow could be used to exploit the phenomenon of thermal rectification [81].

In Fig. 7(d) we plot κ_{xy} versus E_F for $T = 200$ K. We notice the thermal broadening of the ATHC due to the Fermi distributions. Note also that κ_{xy} is suppressed for lower light intensity.

C. Robustness of the topological responses

The results for the topological responses σ_{xy} , α_{xy} , κ_{xy} , and M presented above in the BI and CI phases depend strictly on the parameter $\Delta_1 = \Delta + \alpha \tilde{A}^2/2$ and the value of the mass m . Focusing on Δ_1 first, these responses exhibit a robust pattern of behavior in the BI and CI phases as long as $\Delta_1 > 0$ and $\Delta_1 < 0$ (with $|m| < |\eta|k_D$), respectively. However, varying either Δ or $\tilde{A}$ or both in a way that makes Δ_1 smaller leads to larger magnitudes of α_{xy} and κ_{xy} . This is due to the fact that the band gap depends on Δ_1 ; a smaller Δ_1 leads to a smaller band gap, which generates larger Berry curvature. Consequently, α_{xy} and κ_{xy} are enhanced. We remark that for $\Delta = 0$, the parameter $\Delta_1 = \alpha \tilde{A}^2/2 > 0$ and the SD system is in the BI phase with $C = 0$. Focusing now on the value of $|m|$ (with $\Delta_1 < 0$), the topological responses are enhanced when $|m|$ approaches an SSDC gapless state; see Fig. 2(e). As $|m|$ increases for fixed $\tilde{A}$ and approaches the phase boundaries, $|m| \rightarrow |\eta|k_D$, the band gap reduces and $\Omega(\mathbf{k})$ increases, leading to larger α_{xy} and κ_{xy} .

D. Charge conductivities σ_{xx} and σ_{yy}

We start with the evaluation of the density of states (DOS) and then proceed with the charge conductivities σ_{xx} and σ_{yy} . In this and the following sections, we set $m = 0$.

Density of states. To avoid difficulties associated with the anisotropic energy dispersion, we transform coordinates from (k_x, k_y) to new variables (q_x, q_y) defined by $q_x = \Delta_1 + \alpha k_x^2$ and $q_y = \gamma k_y$. The Jacobian of this transformation is given by [82]

$$J(q, \theta) = \frac{1}{2\gamma\sqrt{\alpha}} (q \cos \theta - \Delta_1)^{-1/2}, \quad (30)$$

where $\tan \theta = q_y/q_x$ and $q = (q_x^2 + q_y^2)^{1/2}$. The DOS $D(E)$ can then be obtained from

$$D(E) = \frac{1}{(2\pi)^2} \int d^2 q J(q, \theta) \delta(E_{\lambda q} - E), \quad (31)$$

where $E_{\lambda q} = \lambda[q^2 + (\eta^2/\alpha)(q \cos \theta - \Delta_1)]^{1/2}$. We have evaluated the integral both numerically and analytically. In the analytical evaluation, we made the approximation $-v \cos \theta + (E^2 + \mu)^{1/2} \simeq (E^2 + \mu)^{1/2}$, where $v = \eta^2/2\alpha$ and $\mu = \eta^2 \Delta_1/\alpha$, which is valid for low light intensities. We find that the results agree extremely well with the numerical ones.

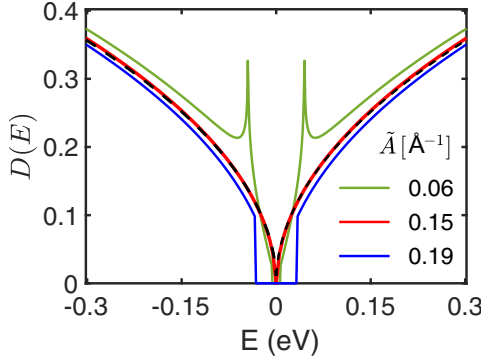


FIG. 8. Density of states $D(E)$ in units of D_0 for increasing values of the light intensity $\tilde{A}$. For $\tilde{A} = 0.06 \text{ \AA}^{-1}$ ($\Delta_1 < 0$) $D(E)$ exhibits van Hove singularities, whereas for $\tilde{A} = 0.19 \text{ \AA}^{-1}$ ($\Delta_1 > 0$) it exhibits jump discontinuities. At the SD transition point ($\tilde{A} = 0.15 \text{ \AA}^{-1}$, $\Delta_1 = 0$) $D(E)$ varies as $\sqrt{E}$. The black dashed line is the approximate analytical result Eq. (34) for $\tilde{A} = 0.15 \text{ \AA}^{-1}$.

Small deviations occur in the case $\Delta_1 < 0$ for very low energies. For $\Delta_1 < 0$, we find

$$D(E) = \frac{D_0|E|}{\sqrt{\epsilon - \Delta_1}} K(r), \quad \sqrt{|\mu|} < |E| < |\Delta_1|, \quad (32)$$

$$D(E) = \frac{D_0|E|}{\sqrt{2\epsilon}} K(1/r), \quad |E| > |\Delta_1|, \quad (33)$$

where $K(x)$ is the complete elliptic integral of the first kind [83], $\epsilon = (E^2 + \mu)^{1/2}$, $D_0 = \sqrt{2m}/2\pi^2\hbar^2 v_y$, and $r = [2\epsilon/(\epsilon - \Delta_1)]^{1/2}$. At the SD transition point, $\Delta_1 = 0$, we find

$$D(E) = \frac{D_0|E|}{\sqrt{2\epsilon}} K(1/\sqrt{2}), \quad (34)$$

where $K(1/\sqrt{2}) = 1.85$. Above the transition point, $\Delta_1 > 0$, we find

$$D(E) = 0, \quad |E| < \Delta_1, \quad (35)$$

$$D(E) = \frac{D_0|E|}{\sqrt{2\epsilon}} K(1/r), \quad |E| > \Delta_1. \quad (36)$$

In Fig. 8 we show $D(E)$ in units of D_0 for an irradiated SD system in the semimetallic phase with two gapped Dirac nodes (green line, $\Delta_1 < 0$), in the SD transition point (red line, $\Delta_1 = 0$), and in the BI phase (blue line, $\Delta_1 > 0$). Here we have used $\omega = 5 \times 10^{15} \text{ Hz}$, $\Delta = -30 \text{ meV}$, and a left-circularly polarized light ($\phi = \pi/2$). For $\Delta_1 < 0$ we notice that $D(E)$ exhibits van Hove singularities at $|E| = |\Delta_1|$ due to saddle points of the energy dispersion; for nonirradiated SD systems [50] they occur at $|E| = |\Delta|$. For $\Delta_1 = 0$, $D(E)$ is $\sim \sqrt{E}$. For $\Delta_1 > 0$, $D(E)$ exhibits a jump at $|E| = \Delta_1$ and increases $\sim \sqrt{E}$ thereafter. We also show the approximate analytical result for the case $\Delta_1 = 0$ by the black dashed line. For the other cases (not shown here) we also find very good agreement with the numerical results.

Charge conductivities. Using the Boltzmann transport theory in the relaxation-time approximation, we obtain the diagonal components of the conductivity tensor as

$$\sigma_{aa} = e^2 \sum_{\lambda=\pm} \int \frac{d^2k}{(2\pi)^2} v_{a,\lambda\mathbf{k}}^2 \tau_{\lambda\mathbf{k}} \left(-\frac{\partial f_{\lambda\mathbf{k}}}{\partial E_{\lambda\mathbf{k}}} \right), \quad (37)$$

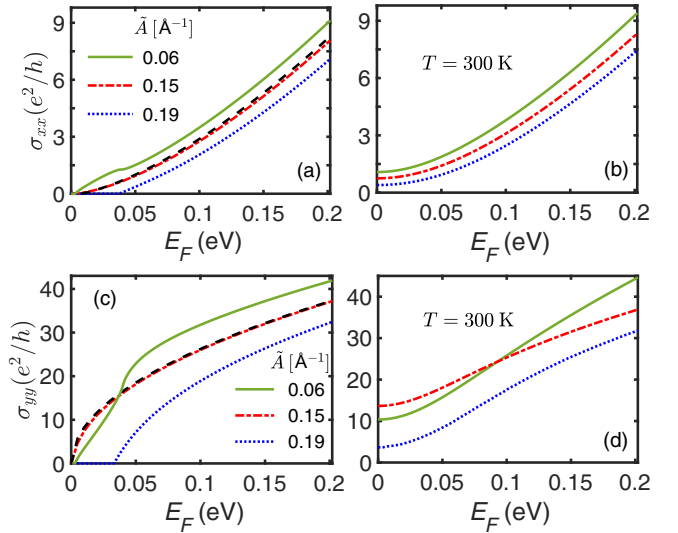


FIG. 9. (a) Charge conductivity σ_{xx} vs E_F for increasing values of the light intensity $\tilde{A}$ and $T = 0 \text{ K}$. The black dashed line is the analytical result Eq. (48) for the SD transition point. (b) The same as in (a) but for $T = 300 \text{ K}$. (c) Charge conductivity σ_{yy} vs E_F for increasing values of $\tilde{A}$ and $T = 0 \text{ K}$. The black dashed line is the analytical result Eq. (49). (d) The same as in (c) but for $T = 300 \text{ K}$.

where $a = x, y$, $\tau_{\lambda\mathbf{k}}$ is the relaxation time, and $v_{a,\lambda\mathbf{k}} = \hbar^{-1} \partial_{k_a} E_{\lambda\mathbf{k}}$ are the band velocities. For the sake of simplicity, we will treat $\tau_{\lambda\mathbf{k}}$ as independent of momentum, $\tau_{\lambda\mathbf{k}} = \tau_F$. The band velocities are easily found to be

$$v_{x,\lambda\mathbf{k}} = \lambda \hbar^{-1} \epsilon_{\mathbf{k}}^{-1} (2\alpha^2 k_x^3 + \Lambda k_x), \quad (38)$$

$$v_{y,\lambda\mathbf{k}} = \lambda \hbar^{-1} \epsilon_{\mathbf{k}}^{-1} \gamma^2 k_y, \quad (39)$$

where $\Lambda = 2\alpha\Delta_1 + \eta^2$, and $\epsilon_{\mathbf{k}}$ is given in Eq. (9) with $m = 0$. We have evaluated numerically the above integrals for zero and finite temperatures (see Fig. 9). However, using the approximation $-\partial f_{\lambda\mathbf{k}}/\partial E_{\lambda\mathbf{k}} \simeq \delta(E_{\lambda\mathbf{k}} - E_F)$, valid for very low temperatures, we obtain analytic expressions for the conductivities when $\Delta_1 = 0$. Transforming (k_x, k_y) to the variables (q, θ) and taking E_F in the electron band, we obtain

$$\sigma_{xx} = \frac{e^2}{h} \frac{\tau_F}{\pi \hbar \gamma \sqrt{\alpha}} \frac{1}{E_F} (I_1 + I_2), \quad (40)$$

where

$$I_1 = \alpha \int (\epsilon_F \cos \theta - \Delta_1)^{5/2} d\theta, \quad (41)$$

$$I_2 = \Lambda \int (\epsilon_F \cos \theta - \Delta_1)^{3/2} d\theta, \quad (42)$$

with $\epsilon_F = (E_F^2 + \mu)^{1/2}$. In obtaining Eq. (40), we made the same approximations as for the DOS. We have also ignored terms $\sim \Lambda^2 \sim \eta^4/\alpha^2$, which are negligible for low light intensities. For σ_{yy} , we obtain

$$\sigma_{yy} = \frac{e^2}{h} \frac{\gamma \tau_F}{4\pi \hbar \sqrt{\alpha}} \frac{\epsilon_F^2}{E_F} I_3, \quad (43)$$

where

$$I_3 = \int \sin^2 \theta (\epsilon_F \cos \theta - \Delta_1)^{-1/2} d\theta. \quad (44)$$

For the SD transition point, $\Delta_1 = 0$, the integrals I_1 , I_2 , and I_3 can be computed analytically; the range of θ in this case is $-\pi/2 < \theta < \pi/2$. They are given by

$$I_1 = 2\alpha E_F^{5/2} \int_0^1 x^{5/2} (1-x^2)^{-1/2} dx = 2\alpha c_1 E_F^{5/2}, \quad (45)$$

$$I_2 = 2\Lambda E_F^{3/2} \int_0^1 x^{3/2} (1-x^2)^{-1/2} dx = 2\Lambda c_2 E_F^{3/2}, \quad (46)$$

$$I_3 = 2E_F^{-1/2} \int_0^1 x^{-1/2} (1-x^2)^{1/2} dx = c_3 E_F^{-1/2}, \quad (47)$$

where $c_1 = 0.7189$, $c_2 = 0.874$, and $c_3 = 3.496$. With the help of Eqs. (45)–(47), we can finally express the charge conductivities as

$$\sigma_{xx} = \frac{e^2}{h} \frac{2\tau_F}{\pi \hbar \gamma \sqrt{\alpha}} (\alpha c_1 E_F^{3/2} + \eta^2 c_2 E_F^{1/2}), \quad (48)$$

$$\sigma_{yy} = \frac{e^2}{h} \frac{\gamma \tau_F}{4\pi \hbar \sqrt{\alpha}} c_3 E_F^{1/2}. \quad (49)$$

We notice that, in the absence of light, $\eta = 0$, the power-law dependence of σ_{xx} on E_F is given by $\sigma_{xx} \sim E_F^{3/2}$. The light manifests in the second term of Eq. (48). On the other hand, $\sigma_{yy} \sim E_F^{1/2}$ independent of the light.

In Figs. 9(a) and 9(c), we show numerical results for σ_{xx} and σ_{yy} , respectively, as functions of E_F for $T = 0$ K and the same parameter values as in Fig. 8. We have used $\tau_F = 160$ fs, which is relevant for a monolayer black phosphorus [84]. We notice that the conductivities exhibit a distinct dependence on E_F . In the gapped semimetallic phase (green solid line, $\Delta_1 < 0$) we notice a change in slope for both σ_{xx} and σ_{yy} near the van Hove singularity, i.e., for $E_F \simeq (|\mu| + \Delta_1^2)^{1/2} \simeq 0.04$ eV (see Fig. 8). For $E_F < (|\mu| + \Delta_1^2)^{1/2}$, both conductivities increase linearly, but the slope of σ_{yy} is approximately ten times greater; this is a manifestation of the linear energy dispersion in k_y . In fact, we notice from Eqs. (48) and (49) that, in the absence of light, $\sigma_{xx}/\sigma_{yy} = (4c_1/mv_y^2 c_3) E_F \sim E_F$, which can be very small, especially for low doping levels. This is a consequence of the much larger square velocity v_y^2 in the direction with linear dispersion compared to v_x^2 . In the absence of light, Eqs. (38) and (39) become $v_x^2 = 4\alpha E_F/\hbar^2$ (for $k_y = 0$) and $v_y^2 = \gamma^2/\hbar^2 = \text{const}$ (for $k_x = 0$) yielding $v_x^2/v_y^2 = (2/mv_y^2) E_F \sim E_F$ [85].

For the SD point ($\Delta_1 = 0$), besides the numerical results (red dashed-dotted lines), we also plot the analytical results (black dashed lines) from Eqs. (48) and (49), finding that the latter is an excellent approximation. In this case, σ_{xx} increases superlinearly but $\sigma_{yy} \sim E_F^{1/2}$. In Figs. 9(b) and 9(d) we show σ_{xx} and σ_{yy} , respectively, for $T = 300$ K. We notice that, for low values of E_F , the finite temperature raises the values of the conductivities. We also notice that the change in slope for $T = 0$ K is smoothed out due to the thermal broadening. We remark that these results are independent of the polarization of the light because of the occurrence of η^2 in the band velocities. This is in contrast to the transverse (topological) responses, where $\Omega(\mathbf{k})$ depends linearly on η .

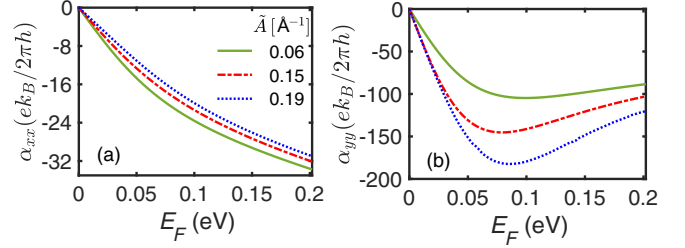


FIG. 10. Thermoelectric conductivities (a) α_{xx} and (b) α_{yy} vs E_F for increasing values of the light intensity $\tilde{A}$. The temperature is $T = 300$ K.

E. Thermoelectric conductivities α_{xx} and α_{yy}

We obtain the diagonal components of the thermoelectric conductivity tensor as

$$\alpha_{aa} = \frac{-e}{T} \sum_{\lambda=\pm} \int \frac{d^2k}{(2\pi)^2} v_{a,\lambda\mathbf{k}}^2 \tau_{\lambda\mathbf{k}} (E_{\lambda\mathbf{k}} - E_F) \left(-\frac{\partial f_{\lambda\mathbf{k}}}{\partial E_{\lambda\mathbf{k}}} \right), \quad (50)$$

where $\alpha = x, y$. We show numerical results for α_{xx} and α_{yy} versus E_F in Figs. 10(a) and 10(b), respectively, for $T = 300$ K. The parameter values are the same as in Fig. 9. In general, the thermoelectric conductivity tensor α_{aa} is proportional to the negative derivative of the charge conductivity tensor σ_{aa} with respect to the chemical potential, $\alpha_{aa} \sim -\partial\sigma_{aa}/\partial E_F$. In the limit $E_F \rightarrow 0$, we notice that $\alpha_{aa} = 0$; the variation in σ_{aa} caused by an infinitesimal shift in E_F vanishes; see Figs. 9(b) and 9(d). As E_F increases, $|\alpha_{xx}|$ increases because the variation in σ_{xx} becomes nonzero. However, the corresponding rate of increase of $|\alpha_{yy}|$ is at least five times larger than $|\alpha_{xx}|$; the slope of σ_{yy} is much greater than that of σ_{xx} . This leads to values of $|\alpha_{yy}|$ that are an order of magnitude larger than those of $|\alpha_{xx}|$. For higher values of E_F , $|\alpha_{yy}|$ tends to a constant value $|\alpha_{yy}| \simeq 100 \text{ ek}_B/2\pi\hbar \simeq 53 \text{ nA/K}$.

We also notice that the effect of the light on the two thermoelectric responses is different. Even though α_{xx} depends weakly on the light intensity $\tilde{A}$, it is nevertheless suppressed as $\tilde{A}$ increases. Its highest values are attained when the SD system is in the gapped semimetallic phase, $\tilde{A} = 0.06 \text{ \AA}^{-1}$. In contrast, α_{yy} depends strongly on the light intensity and it is enhanced as $\tilde{A}$ increases; its highest values are attained in the BI phase, $\tilde{A} = 0.19 \text{ \AA}^{-1}$. For $E_F = 0.8$ eV and $\tilde{A} = 0.19 \text{ \AA}^{-1}$, we estimate their values to be $\alpha_{xx} \simeq -9 \text{ nA/K}$ and $\alpha_{yy} \simeq -97 \text{ nA/K}$.

F. Thermal conductivities κ_{xx} and κ_{yy}

We obtain the diagonal components of the thermal conductivity tensor as

$$\kappa_{aa} = \frac{-1}{T} \sum_{\lambda=\pm} \int \frac{d^2k}{(2\pi)^2} v_{a,\lambda\mathbf{k}}^2 \tau_{\lambda\mathbf{k}} (E_{\lambda\mathbf{k}} - E_F)^2 \left(-\frac{\partial f_{\lambda\mathbf{k}}}{\partial E_{\lambda\mathbf{k}}} \right), \quad (51)$$

where $\alpha = x, y$. In Figs. 11(a) and 11(b) we show the thermal conductivities κ_{xx} and κ_{yy} , respectively, as functions of E_F for $T = 300$ K, and for the same parameter values as in Fig. 9. Their dependence on E_F is similar to those of the charge

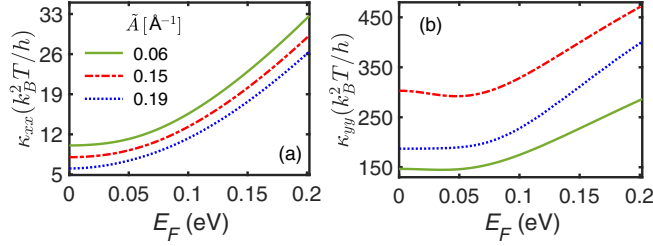


FIG. 11. Thermal conductivities (a) κ_{xx} and (b) κ_{yy} vs E_F for increasing values of the light intensity $\tilde{A}$. The temperature is $T = 300$ K.

conductivities. Similarly to the thermoelectric conductivities, we notice that the dependence of κ_{yy} on the light intensity $\tilde{A}$ is much stronger than that of κ_{xx} . We remark that κ_{yy} can be two orders of magnitude larger than κ_{xx} . For $E_F = 0$ and $\tilde{A} = 0.15 \text{ \AA}^{-1}$, we estimate their values to be $\kappa_{xx} \simeq 6.9 \times 10^{-10} \text{ W/K}$ and $\kappa_{yy} \simeq 2.6 \times 10^{-8} \text{ W/K}$.

VI. POSSIBLE OPTOTHERMOELECTRIC APPLICATIONS

The reversal of the direction of flow of the anomalous (topological) currents by flipping the polarization of light is promising for possible optothermoelectric applications and devices. For instance, the reversal and control of the ATHC κ_{xy} with light suggests a possible pathway for the exploitation of the phenomenon of thermal rectification [81], which is desirable in quantum [86] and magnetic [87] thermal transistors. The former are analogous to electronic transistors with temperatures replacing voltages and thermal energy replacing electric current. The latter use a temperature-dependent magnetization of a ferromagnetic material to control the source-drain heat flow by a gate temperature in a manner that leads to heat flow switching. Our results suggest that heat flow switching could be achieved in irradiated Dirac or semi-Dirac materials by changing the polarization of light, which leads to a sign change of the Berry curvature—the driver of the anomalous topological responses.

The light-induced sign change of the Berry curvature also leads to a sign reversal of the Nernst signal $\mathcal{N} = E_y / \nabla_x T = (\alpha_{xy}\sigma_{xx} - \alpha_{xx}\sigma_{xy}) / (\sigma_{xx}^2 + \sigma_{xy}^2)$. Switching the polarization of light results to a sign change of α_{xy} and of σ_{xy} , with α_{xx} and σ_{xx} remaining unchanged. This leads to a reversal of the polarity of $\mathcal{N}$, which could be useful for switchable transverse thermoelectric generation [88] without using magnetic materials.

VII. SUMMARY AND CONCLUSIONS

We investigated the topological phase transitions in a semimetallic SD material under the application of off-resonant light and with an inversion symmetry breaking mass. We derived analytical expressions for the energy spectrum, the Berry curvature, the Chern numbers, and we presented the $(m, \tilde{A})$ phase diagram. We also showed the existence of single semi-Dirac-cone semimetal states. These remarkable states emerge along the phase boundaries; a hallmark of them is that one SD cone is gapless and the other is gapped. We showed that, as the light intensity increases for fixed mass, the system undergoes normal-Chern-normal insulator phase

transitions. At finite temperatures, thermal averaging or dephasing to mixed states results in a deviation from an integer Chern number. We have evaluated the thermal Uhlmann number and showed that the CI phase is stable for temperatures $\lesssim 30$ K.

The TRS breaking light induces and controls the Berry-phase mediated anomalous thermoelectric responses in SD materials. In particular, we investigated the anomalous Nernst (α_{xy}) and thermal Hall (κ_{xy}) conductivities, and the orbital magnetization M . In the BI phase, we find that α_{xy} versus E_F exhibits a dip (peak) at the valence-band (conduction-band) edge. The dip-peak profile is reversed when the light intensity drives the system to the CI phase. We also showed that switching the light's circular polarization, from left to right, induces a sign reversal in M , σ_{xy} , α_{xy} , and κ_{xy} . Physically this allows us to reverse the direction of flow of the transverse thermoelectric charge current and that of the heat current.

We have also investigated the diagonal components of the charge, thermoelectric, and thermal conductivity tensors, σ_{aa} , α_{aa} , and κ_{aa} , respectively, with $a = x, y$. We find that σ_{yy} , α_{yy} , and κ_{yy} depend strongly on the light intensity compared to those in the x direction. Additionally, we showed that the values of α_{yy} and κ_{yy} are one and two orders of magnitude larger than α_{xx} and κ_{xx} , respectively. We also find that the light has the opposite effect on α_{xx} and α_{yy} ; as $\tilde{A}$ increases, $|\alpha_{xx}|$ decreases but $|\alpha_{yy}|$ increases. These results may be promising for light-induced caloritronic applications.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX: GAP ORIGINATING FROM THE MASS m

A local on-site staggered sublattice potential in honeycomb lattices breaks the equivalence between A and B sites, and therefore also breaks the inversion symmetry [89]. It is expressed as

$$h_s = \sum_{\mathbf{r}_A} E_A c_A^\dagger(\mathbf{r}_A) c_A(\mathbf{r}_A) + \sum_{\mathbf{r}_B} E_B c_B^\dagger(\mathbf{r}_B) c_B(\mathbf{r}_B), \quad (\text{A1})$$

where E_A and E_B are the orbital energies on sites A and B , respectively. This local perturbation term is nondispersive, and its Bloch Hamiltonian in $\mathbf{k}$ space is written as

$$h_s(\mathbf{k}) = h_s = m_0 \sigma_0 + m \sigma_z, \quad (\text{A2})$$

where the first term with $m_0 = (E_A + E_B)/2$ can be absorbed in the chemical potential E_F and is ignored. The second term

with $m = (E_A - E_B)/2$ is parity breaking and opens a gap of size $2|m|$ at the Dirac points. Such a gap has been demonstrated in epitaxial graphene [90].

A honeycomb lattice can also exhibit SD dispersion when the particle hopping is different along different directions of the lattice, thus breaking the rotational symmetry. An example is graphene deformed by applying a uniaxial strain in one direction [50]. We remark that, for such a semi-Dirac honeycomb lattice, direct evidence of the anisotropic transport of polaritons has been reported [43]. To generate a mass for the SD fermions, one possibility is to use deformed graphene on a substrate that makes the A and B sites inequivalent as a result of the interlayer interaction. A possible choice for a substrate is hexagonal boron nitride (h -BN). It has been demonstrated that, for isotropic graphene placed on top of BN, the mass

generated is $m \simeq 26$ meV [90]. For SD deformed graphene, the interaction with the substrate will be weaker and the expected value of the mass should be lower. However, it has proved challenging to realize the SD dispersion in these systems.

Other honeycomb materials, such as silicene and germanene, were shown to host the SD semimetal phase with the application of structural strain and the addition of oxygen atoms to modify the hopping energies [91]. Due to the buckled structure, the two sublattice planes of silicene [92] are separated by a distance $d = 0.46$ Å. The application of an electric field E_z perpendicular to the plane generates a staggered sublattice potential with $m = E_z d/2$. In this case, for $E_z = 10$ meV/Å we estimate that $m \simeq 2.3$ meV and the gap $\simeq 4.6$ meV.

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