Direction dependent giant optical conductivity in 2D semi-Dirac materials

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Using linear response theory, we evaluate the optical conductivity of 2D semi-Dirac materials for light polarized along two mutually orthogonal directions and predict a strong anisotropy of the optical response as a consequence of their unique dispersion spectrum. Our results also predict a large degree of sensitivity for inter-band optical conductivity to the polarization direction. While it reveals an abruptly large value for certain frequency for light along a particular polarization direction, it is significantly suppressed along the direction orthogonal to the former. The frequency corresponding to the predicted giant optical conductivity is found to be independent of the chemical potential, for a lightly doped system. This direction-dependency of the giant inter-band optical conductivity may in turn be used to uniquely predict the dispersive nature of the 2D semi-Dirac materials, in addition to possible applications that arise from this direction dependent optical transparency.

Low energy excitations with massless Dirac particle behavior are characteristics of some illustrious 2D and quasi-2D materials such as graphene, silicene, MoS$_2$, 8-\textit{Pmmn} borophene, to name a few. Topological insulator states in 2D based on a honeycomb lattice, induced by spin-orbit energy gap also host Dirac-like edge states\cite{23-25}. Several attempts were also successful to induce spin-orbit energy gap in 3D materials so as to yield such Dirac-like surface states\cite{14}. The massless Dirac particles have a low energy band dispersion, which is linear in all \textit{k}-space directions (also known as Dirac cone), with particle and hole states lying respectively above and below a nodal point called the Dirac node. To describe such states, the term Dirac semi-metal is often used.

The Dirac-cone in the dispersion spectrum controls the various low energy properties such as specific heat\cite{6,17} suppression of back-scattering\cite{18,19}, transport properties such as optical conductivity\cite{20} and magnetic field responses of such 2D materials. Also, exotic properties like quantum Hall effect have been revealed by semi-metallic Dirac materials like graphene even at room temperature\cite{21}. Several theoretical proposals of quantum Hall effect were also predicted in other 2D Dirac materials such as borophene\cite{38}, and MoS$_2\text{Pmmn}$\cite{15}, to name a few. Recently, a distinct class of 2D Dirac materials called semi-Dirac (SD) materials has been discovered in materials or systems such as TiO$_2$/V$_2$O$_3$ nanostructure\cite{22}, BEDT-TTF$_2$I$_3$ salt under pressure\cite{23}, hexagonal lattices in the presence of a magnetic field\cite{24} and dielectric photonic systems\cite{25}. This class of materials has a unique low energy dispersion, which is quadratic in a given direction and linear in an orthogonal direction with respect to the former.

The complex frequency-dependent optical conductivity is the sum total of the inter-band, arising from the particle-hole transitions and the dynamic Drude conductivity, due to the intra-band transitions. The real part of the complex optical conductivity is directly tied to the absorption of the incident photon energy. Its measurement is one of the important tools for extracting the shape and nature of the material’s band dispersion. The optical conductivity has been extensively studied in various 2D-Dirac materials, ranging from graphene\cite{26}\cite{29}, silicene\cite{30}\cite{32}, MoS$_2\text{Pmnn}$\cite{33}, 8-\textit{Pmmn} borophene\cite{34} to the surface states of topological insulator\cite{35}\cite{36}. Its results carry information of the uniqueness of the material’s dispersive nature.

Besides the above, the search for transparent conductors has attracted much interest in fundamental research and for the technological development of optoelectronic devices. Graphitic materials through lithium intercalation\cite{37} and multilayer graphene in bromine-intercalated graphite\cite{38} which both show a very high transmission rate further pave way in the direction towards research of transparent conductors. In this context, this paper makes an important prediction that SD materials possess a very high degree of anisotropy of the optical conductivity. This, in turn, suggests that such materials should show a relatively different degree of optical transmission along different directions. It makes it even more interesting that in one particular direction, at a particular light frequency, the optical transmission is almost blocked.

The low energy Hamiltonian that features a band dispersion in SD materials goes as:\cite{39,40}

$$H_0 = \mathbf{g}(\mathbf{k}) \cdot \mathbf{\sigma},$$

where \( \mathbf{g}(\mathbf{k}) \equiv (\alpha \mathbf{k}^2 - \delta_0, \nu \mathbf{k}_y) \) with \( \delta_0 \) and \( \alpha \) being the related system parameters and \( \mathbf{\sigma} \equiv (\sigma_x, \sigma_y) \) are the 2 \times 2 Pauli’s matrices. Also, a term Type-I SD for the above Hamiltonian was coined by Huang, \textit{et. al.}\cite{39} which differs from another type-II SD Hamiltonian since the later also shows signature of Chern insulating state. The later described very well the emergence of Chern insulating states in super-crystal (TiO$_2$)$_5$/\textit{(VO}_2\text{)}$_2$\cite{41}. In this paper we refer only to the type-I SD Hamiltonian. The eigensystem of \( H_0 \) is \( \varepsilon_{\lambda}(\mathbf{k}) = \lambda \sqrt{g_{\perp}^2 + g_{\parallel}^2} \) and \( \psi_{\lambda}^{\mathbf{k}}(r) = \frac{e^{i \mathbf{k} \cdot \mathbf{r}}}{\sqrt{2}} \left( 1, \frac{\mathbf{i} \lambda - i \delta_0 + \nu \mathbf{k}_y}{\sqrt{g_{\perp}^2 + g_{\parallel}^2}} \right)^T \), respectively, where \( \lambda = +/- \) denotes the conduction/valence bands and \( T \) denotes the transpose. The energy separation between the valence and conduction bands is denoted by \( \Delta_{\mathbf{k}} = \varepsilon_+(\mathbf{k}) - \varepsilon_-(\mathbf{k}) = 2\sqrt{g_{\perp}^2 + g_{\parallel}^2} \).

In comparison to some conventional 2D Dirac materials, for example graphic, the band dispersion in SD...
materials also features a gap-less system, but with two Dirac nodes located exactly at \((k_x, k_y) = (\pm k_0, 0)\), where \(k_0 = \sqrt{\hbar B/\alpha}\), such that the two Dirac nodes are separated by \(2k_0\) in the momentum space. The electron and hole states are degenerated at the two Dirac points and are separated by a gap \(\Delta_k\) elsewhere. The plot of the band dispersion relation with respect to \(\omega\) is shown in Fig. 1(a). By virtue of such Dirac cones dispersion, they are expected to possess low energy transport properties that are unique in comparison to their counterpart 2D materials with conventional Dirac cone. For example, the energy of the Landau levels varies with the magnetic field, \(B\) as \((n + 1/2)B^{2/3}\) while it varies as \(\sqrt{nB}\) in the case of graphene\(^{34,35}\). Over and above, the investigation of the optical conductivity in SD materials should lead to some new interesting physics by virtues of such Dirac cones dispersion. The vertical green lines in Fig. 1(a & b) depict the possible particle-hole direct transitions from \(\varepsilon_\pm(k)\) to \(\varepsilon_\pm(k)\) with conserved momentum vector. One can easily identify the avalanches of \(k\)-states available for particle-hole transitions in between particle states with energy \(\varepsilon_+\) and hole states with energy \(\varepsilon_-\), with \(\varepsilon_\pm - \varepsilon_\pm (k = 0)\) (part (iii) of Fig. 1(b)). This will result in an abruptly large inter-band joint density of states when \(\Delta_k = 0\) (Fig. 1(c)).

In this paper, we study mostly the inter-band optical conductivity of SD materials. The abruptly large inter-band joint density explained above dictates the giant inter-band optical conductivity when light is polarized along a direction where the dispersion is linear. The frequency that excites this giant optical conductivity exactly equals to the energy separation between the particle and hole states at the \(k = 0\) point, which entirely depends on the band parameters of the SD materials. Such giant optical conductivity was also discovered in three-dimensional topological Dirac semi-metals\(^{41,42}\) where the very large optical response was explained explicitly based on the electron-hole transition across the Fermi arc contours, which is one of the signatures of topological Weyl semi-metals. We investigate the optical conductivity of SD materials in the low and high-frequency regime considering light with both the \(x\)- and \(y\)-polarization states. The main finding of this paper is centered around the giant inter-band optical conductivity along the \(y\) direction which may serve as an important signature of the SD materials. Also, the high degree of anisotropy of optical conductivity suggested that the SD materials can be a potential candidate of transparent conductor along one particular direction while bearing a very high absorption rate along the orthogonal direction.

We consider a SD materials subjected to zero-momentum electric field \(\mathbf{E} \sim \mathbf{v}_\omega e^{i\omega t} (\mathbf{v} = \hat{x}, \hat{y})\) with oscillation frequency \(\omega\). The total charge optical conductivity tensor is given by the relation \(\Sigma_{\nu\mu}(\omega) = \delta_{\nu\mu} \sigma_D(\omega) + \sigma_{\nu\mu}(\omega)\), \(\sigma_D(\omega) = \sigma_d/(1 - i\omega\tau)\) is the dynamic Drude conductivity due to the intra-band transitions, with \(\sigma_d\) being the static Drude conductivity and \(\sigma_{\nu\mu}(\omega)\) is the complex optical conductivity due to inter-band transitions between particle and hole states.

**Inter-band optical conductivity:** Now, we calculate the inter-band optical conductivity for light which is polarised along both the \(x\) and \(y\)-directions. Within the framework of linear response theory, the Kubo formula
responding Green’s function is given by

$$\sigma_{\nu\nu}(\omega) = i\frac{e^2}{\pi\varepsilon_0 \hbar^2} \int d\mathbf{k}$$

$$T \sum_n \text{Tr}(\hat{v}_\nu \hat{G}(\mathbf{k}, \omega_n) \hat{v}_\nu \hat{G}(\mathbf{k}, \omega_n + \omega)) \delta_{\omega_n, \omega+n+i\delta}. \quad (2)$$

Here $T$ is the temperature and $\omega_l = (2l+1)\pi T$ and $\omega_n = 2n\pi T$ are the fermionic and bosonic Matsubara frequencies, respectively, with $n$ and $l$ being integers.

In general, we will also consider the effect of the perturbation that opens up a gap at the two Dirac nodes. Thus the total hamiltonian is $H = H_0 + \delta H$, where $\delta H = m_0 \sigma_z$. With respect to this Hamiltonian, the corresponding Green’s function is

$$\hat{G}(\mathbf{k}, \omega) = \frac{1}{2} \sum_{\lambda} \left[ \sigma_0 + \lambda \frac{\mathbf{F} \cdot \sigma}{\sqrt{m_0^2 + g_y^2 + g_x^2}} \right] G(\mathbf{k}, \omega),$$

(3)

where $\sigma_0$ is the unit 2 × 2 matrix, $\mathbf{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the $x$, $y$ and $z$-components of Pauli’s matrix and the vector $\mathbf{F} \equiv (F_x, F_y, F_z)$ are given by

$$(F_x, F_y, F_z) = \frac{\lambda(k_x^2 - \delta_0, \lambda(k_y, \mu_0, m_0))}{\sqrt{(v(k_y)^2 + m_0^2 + (\lambda(k_x^2 - \delta_0)^2)}}$$

(4)

with $G_\lambda(\mathbf{k}, \omega) = [i\hbar \omega + \mu - \varepsilon(\mathbf{k})]^{-1}$. With the above Green’s function in Eq. (3), the following quantity, $\text{Tr}(\hat{v}_\nu \hat{G}(\mathbf{k}, \omega_n) \hat{v}_\nu \hat{G}(\mathbf{k}, \omega_n + \omega))$ is obtained as

$$\text{Tr}(\hat{v}_\nu \hat{G}(\mathbf{k}, \omega_n) \hat{v}_\nu \hat{G}(\mathbf{k}, \omega_n + \omega)) = 2 \left( \frac{\hbar}{\pi} \right)^2 \sum_{\lambda, \lambda'} \left[ 1 - \lambda' \left( F_x^2 - F_y^2 + F_z^2 \right) \right] G(\mathbf{k}, \omega_n) G(\mathbf{k}, \omega_n + \omega).$$

Using the following Matsubara frequency summation identity

$$T \sum_n \left[ \frac{1}{i\hbar \omega_n + \mu - \varepsilon(\mathbf{k})} \right] \frac{1}{1 - \varphi(\mathbf{k} - \mathbf{k'})} \begin{cases} \frac{f(\varepsilon(\mathbf{k})) - f(\varepsilon(\mathbf{k}'))}{i\hbar \omega_n - \varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k})}, & \text{if } \lambda \neq \lambda' \\ 0, & \text{otherwise}, \end{cases}$$

(5)

with $f(\varepsilon) = 1/(\exp[\beta(\varepsilon - \mu)] + 1)$ being the fermi Dirac distribution function, $\mu$ is the chemical potential and $\beta = 1/k_BT$, one can write

$$T \sum_n \text{Tr}(\hat{v}_\nu \hat{G}(\mathbf{k}, \omega_n) \hat{v}_\nu \hat{G}(\mathbf{k}, \omega_n + \omega_n)) = 2 \left( \frac{\hbar}{\pi} \right)^2 \sum_{\lambda, \lambda'} \left[ 1 - \lambda' \left( F_x^2 - F_y^2 + F_z^2 \right) \right] \frac{f(\varepsilon(\mathbf{k})) - f(\varepsilon(\mathbf{k}'))}{i\hbar \omega_n - \varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k})}.$$ 

For simplicity, we have used the notation $f(\varepsilon(\mathbf{k})) \equiv f(\varepsilon(\mathbf{k}))$. Using the result of the above equation into Eq. (3), we have

$$\sigma_{\nu\nu}(\omega) = \frac{e^2}{i2\pi\omega} \left( \frac{\hbar}{\pi} \right)^2 \int d\mathbf{k} \left[ 1 - \lambda' \left( F_x^2 - F_y^2 + F_z^2 \right) \right] \frac{f(\varepsilon(\mathbf{k})) - f(\varepsilon(\mathbf{k}'))}{i\hbar \omega_n - \varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k})}.$$ 

(6)

The real part of the optical conductivity which is directly tied to the absorptive part is then given by

$$\text{Re} \left[ \sigma_{yy}(\omega) \right] = \frac{e^2}{2\pi\omega} \left( \frac{\hbar}{\pi} \right)^2 \sum_{\lambda, \lambda'} \int d\mathbf{k} \left[ 1 - \lambda' \left( F_x^2 - F_y^2 + F_z^2 \right) \right] \frac{f(\varepsilon(\mathbf{k})) - f(\varepsilon(\mathbf{k}'))}{i\hbar \omega_n - \varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k})}.$$ 

(7)

Therefore finally, we have the expression of $\sigma_{yy}(\omega)$ as follows

$$\text{Re} \left[ \sigma_{yy}(\omega) \right] = \frac{e^2}{2\pi\omega} \left( \frac{\hbar}{\pi} \right)^2 \int d\mathbf{k} \left[ 1 + F_x^2 - F_y^2 + F_z^2 \right] \delta(\omega - \Delta_k).$$ 

(8)

Similarly, the real part of $xx$-component of the optical conductivity can be obtained as

$$\text{Re} \left[ \sigma_{xx}(\omega) \right] = \frac{2e^2}{\pi\omega} \left( \frac{\hbar}{\pi} \right)^2 \int d\mathbf{k} \cos \theta \left[ 1 - F_x^2 + F_y^2 + F_z^2 \right] \delta(\omega - \Delta_k).$$ 

(9)

The integral in Eq. (9 & 10) is then evaluated numerically.

**Drude conductivity:** In order to obtain the total optical conductivity in the entire range of frequency, we
now calculate the static Drude conductivity, that will dominate in the small frequency limit ($\omega \to 0$). In the background of Boltzmann - equation, the Drude conductivity is written as

$$\sigma_{xx}^d = -\frac{1}{(2\pi)^2} \int dk |v_{k\nu}|^2 \frac{\partial f(\epsilon(k))}{\partial \epsilon(k)}, \quad (11)$$

where $v_{k\nu} = \langle \psi_k | \frac{\partial H}{\partial \epsilon_{\nu}} | \psi_k \rangle$ is the band velocity along a direction, $\nu$. For simplicity, in the small temperature limit, one can take the approximation, $-\frac{\partial f(\epsilon(k))}{\partial \epsilon(k)} = \delta(\epsilon(k) - \mu)$ for evaluating $\sigma_{xx}^d$.

Let us now analyze and discuss the behavior of the total optical conductivity taken as derived in Eqs. (9 & 10). For our numerical analyses, we have taken the system parameters for typical SD materials according to Ref. [8] and the references therein. The various parameters are taken as $\alpha = 7.5$ meV nm$^2$, $v = 65$ meV nm, $\delta_0 = 10$ meV. The SOC induced effective mass that opens up a gap, $m_0 = 1$ meV and scattering time, $\tau = 0.04$ ps are taken for illustration purposes.

Firstly, we analyze the inter-band contribution to the optical conductivity given in Eqs. (9 & 10). Without the loss of generality, we will discuss the behavior of optical conductivity for the case of gapped SD system. With the inclusion of perturbation $\delta H = m_0 \sigma_z$, the gap between the valence and conduction bands at the two Dirac points $(k_x, k_y) = (\pm k_0, 0)$ is $2m_0$ and is $\Delta_{k=0} = \varepsilon_+ - \varepsilon_- = 2\sqrt{m_0^2 + \delta_0^2}$ at $k = 0$, where $\varepsilon_+ = \varepsilon_+(k = 0) = \pm \sqrt{m_0^2 + \delta_0^2}$. The limit of $m_0 \to 0$ will yield its behavior for a gap-less system. The plots of the total optical conductivity for both gapped and gapless SD system at three different chemical potential is given in Fig. [2]. We consider only lightly doped system where the chemical potential is always chosen such that $\mu < \Delta_{k=0}$. The inter-band optical conductivity spectrum originates at $\hbar \omega = 2\mu$. For frequency where $\hbar \omega < 2\mu$, all inter-band transitions are Pauli’s blocked. This condition is shown by the Pauli’s blocked transitions indicated by black arrows in Fig. [2(a)]. To initiate the inter-band optical conductivity, the frequency should also be greater than $2m_0$. Again, the frequency for which $\hbar \omega < 2m_0$ corresponds to the unavailable k-states for inter-band optical conductivity. In the regime $\hbar \omega > 2\mu$ there is a smooth variation of its $xx$-component. However, we find that $yy$-component of optical conductivity interestingly, acquires a giant value (several of $e^2/h$) when the frequency of light is such that $\hbar \omega = 2\sqrt{m_0^2 + \delta_0^2} = \Delta_{k=0}$. For proper understanding of such features, we again refer to Fig. [2(b & c)]. In Fig. [2(b)], we have given a general representation of the various transitions in between the electron and hole states with same k-vector magnitude across three types of Fermi contours as shown in Secs. (a) (b) and (c). It is easy to notice the maximum available k-states for the inter-band optical conductivity when the energy difference is closed to $\Delta_{k=0}$ (shown in Sec. (iii) of Fig. [2(b)]). This behaviour will result to a giant optical conductivity at $\hbar \omega = \Delta_{k=0}$ as seen in Fig. [2 & 3]. As expected, the characteristic frequency that excites the giant optical conductivity is independent of the chemical potential as shown in Fig. [3((a) & (b))] by the horizontal yellowish line. The giant optical conductivity $\sigma_{yy}$, implies that there is a huge absorption rate for light of frequency $\hbar \omega = 2\sqrt{m_0^2 + \delta_0^2}$ with $y$-polarization.

We now discuss a more informative way to understand the giant optical conductivity at $\hbar \omega = 2\sqrt{m_0^2 + \delta_0^2}$ from
Given by

\[ \omega = \sqrt{m_0^2 + \delta^2}. \]

with \( \delta \) is the electron-hole states energy separation at \( k_0 \), which thus leads to zero joint density of states in this region and ultimately zero inter-band optical conductivity. The joint density of states is finite in regime II and III. Separating the regime II and III is a yellowish horizontal line with \( \hbar \omega = \Delta_{k=0} \). This line corresponds to the giant optical conductivity which is independent of the chemical potential. This very large joint density of states arises from the van Hove singularity which as indicated in the above discussion, is due to the maximum available \( k \)-value for inter-band transitions in and around \( \hbar \omega = \Delta_{k=0} \).

In conclusions, we have presented detailed theoretical studies of the optical conductivity of 2D semi-Dirac materials. We found that the optical response is highly sensitive to the direction of polarization of light. For light polarized in the direction where the dispersion is linear, our results predict a giant inter-band optical conductivity when the frequency corresponds to the electron-hole states energy separation at \( k = 0 \), while on the other hand, the inter-band optical conductivity is significantly muted when light is polarized along the direction orthogonal with respect to the former. Also, the frequency that excites this giant optical conductivity is found to be independent of the chemical potential for lightly doped semi-Dirac system. The high degree of anisotropy of optical conductivity suggested that the SD materials can be a potential candidate of transparent conductor where there will be transparency along one direction while bearing a very high absorption rate along the orthogonal direction. Also, the direction dependency of this giant inter-band optical conductivity can be presented as a tool that can be uniquely used in order to probe the dispersive nature of 2D semi-Dirac materials. To wind up this paper, we would also proposed the possibility of extracting some interesting physics that may co-exist along with the giant optical conductivity in super-crystal (TiO\(_2\))/((VO\(_2\))\(_3\)) which shows Chern insulating states, where the band dispersion is governed by a “type-II” semi-Dirac dispersion.

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\[ D(\omega) = \frac{1}{4\pi} \sum_\xi \int d\theta [f_+(k_{\omega,\xi}(\theta)) - f_-(k_{\omega,\xi}(\theta))] \times \frac{\delta(k - k_{\omega,\xi}(\theta))}{\frac{\partial}{\partial k} (\hbar \omega - \Delta_k)}_{k_{\omega,\xi}(\theta)}, \]

where \( k_{\omega,\xi}(\theta) \) are the solutions of the equation \( \hbar \omega = \Delta_k \) given by

\[ k_{\omega,\xi}(\theta) = \sec \theta \sqrt{2} \sqrt{\frac{2\delta_0}{\alpha} - \frac{\nu^2}{\alpha^2} \tan^2 \theta \pm \kappa^2}, \]

with \( \kappa^2 = \sqrt{\frac{(\hbar \omega)^2 - 4m_0^2}{\alpha^2} - \frac{\nu^2}{\alpha^2} \left( \frac{4\delta_0}{\alpha} \tan \theta - \frac{\nu^2}{\alpha^2} \tan^2 \theta \right)} \) and the subscript \( \zeta \) goes for \( \pm \) in Eq. (13), which shows that there could be two values of \( k_{\omega,\xi}(\theta) \), say \( k_{\omega,1} \) for “+” and \( k_{\omega,2} \) for “−”. It is easy to see from Fig. [1(c)], that we have both solutions \( k_{\omega,1} \) and \( k_{\omega,2} \) only for \( \hbar \omega < \Delta_{k=0} \), while there is only one possible \( k_{\omega} \) value for \( \hbar \omega > \Delta_{k=0} \).

In Fig. [3(c)], separating the regime I and II is the line \( \hbar \omega = 2\mu \), with \( \hbar \omega >= 2m_0 \). Below this line is region I which includes the parts with all the Pauli’s blocked inter-band transition (basically indicated by black arrows in Fig. [1(a)]), which thus leads to zero joint density of states of this region and ultimately zero inter-band optical conductivity. The joint density of states is finite in regime II and III. Separating the regime II and III is a yellowish horizontal line with \( \hbar \omega = \Delta_{k=0} \). This line corresponds to the giant optical conductivity which is independent of the chemical potential. This very large joint density of states arises from the van Hove singularity which as indicated in the above discussion, is due to the maximum available \( k \)-value for inter-band transitions in and around \( \hbar \omega = \Delta_{k=0} \).

FIG. 3. (a): Gradient plot of \( yy \)-components of conductivity (in units of \( e^2/h \)) from for gapped SD materials which clearly shows that the giant optical conductivity is only excited by frequency \( \hbar \omega = \sqrt{m_0^2 + \delta^2} \). (b) Gradient plot of \( yy \)-components of conductivity (in units of \( e^2/h \)) for gap-less SD materials. (c) Gradient plot of the joint density of state.

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